HIGH-END COMPUTING CAPABILITY PORTFOLIO

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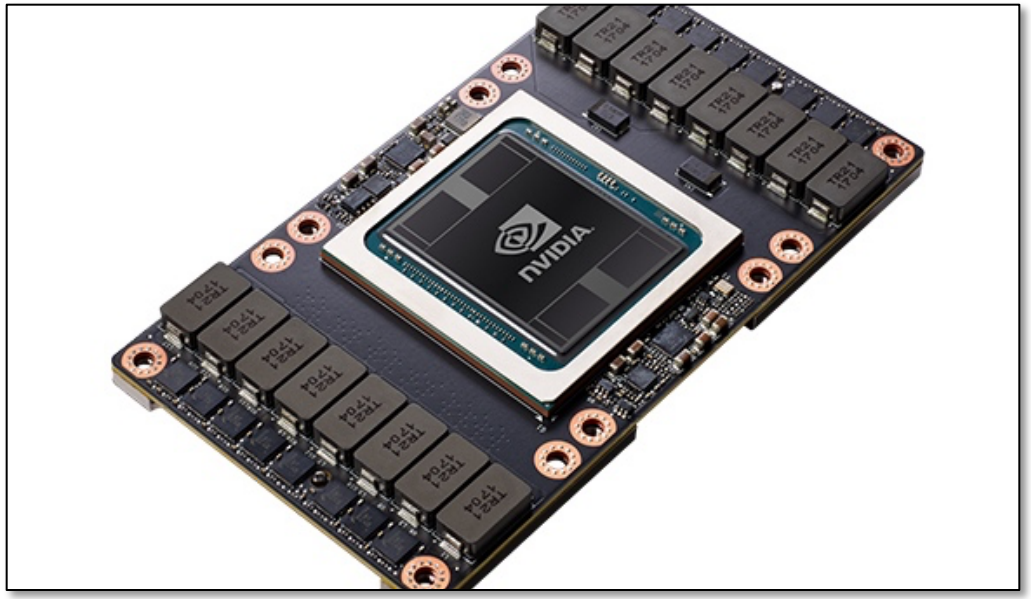
NASA Advanced Supercomputing Division

December 10, 2020

New GPGPU Nodes Released to Users

- Thirty-eight new nodes containing NVIDIA V100 General-Purpose Graphics Processing Units (GPGPUs) were released into production on November 19, 2020.
  - The addition increases the number of V100 nodes (4 GPU cards each) available to users from 19 to 57, for a total of 236 GPGPUs.
  - This expansion marks the second GPU augmentation since the original 64 NVIDIA Tesla K40 nodes were installed in 2015.
- Specific types of scientific workloads can leverage GPGPUs to greatly accelerate performance and enable users to get faster results than they could using traditional CPUs alone.
- HECC users will greatly benefit from the expanded GPGPU capability, as the demand for artificial and machine learning methods continue to grow rapidly within the NASA community.
- A HECC-hosted virtual GPU Hackathon (Sept. 28–Oct. 7) paired developers with computer experts for hands-on porting, optimization, and troubleshooting of applications important for NASA projects.

IMPACT: This expansion triples HECC's V100 GPGPU compute capabilities, enabling further practical uses of artificial intelligence and machine learning by NASA scientists and engineers.



NVIDIA V100 NVLink General-Purpose Graphics Processing Unit (GPGPU). The Pleiades supercomputer was augmented with 38 new V100 nodes, expanding HECC's GPGPU capability. *Image courtesy of NVIDIA*

Newly Expanded Aitken is Successfully Benchmarked

- HECC system administrators ran the LINPACK and HPCG benchmarks on the newly expanded Aitken supercomputer to measure its performance and identify any faulty components prior to releasing the system for general user availability.
  - The system achieved 5.795 petaflops (PF) on the LINPACK benchmark and 113.47 teraflops (TF) on the HPCG benchmark.
  - The Aitken expansion and benchmarking were completed after the submission deadline to the November 2020 TOP500 and HPCG lists. If the results had been included, the system would be ranked #48 in the TOP500 and #33 on the HPCG list.
- These benchmarks, running on the full system also act as diagnostic tests, identified a marginal hardware component that was replaced prior to integration and testing.
- The LINPACK and HPCG benchmarks are widely used to evaluate the performance of different supercomputing systems and provide two complementary viewpoints on how systems perform on different workloads.
- The expansion is currently undergoing integration and testing and is expected to be ready for general use in January 2021.

IMPACT: HECC regularly upgrades its resources to meet NASA's increasing supercomputing requirements and increase science and engineering results. Running the LINPACK and HPCG benchmarks on expanded systems provides a good method to identify and address system issues, thereby improving overall reliability for users.

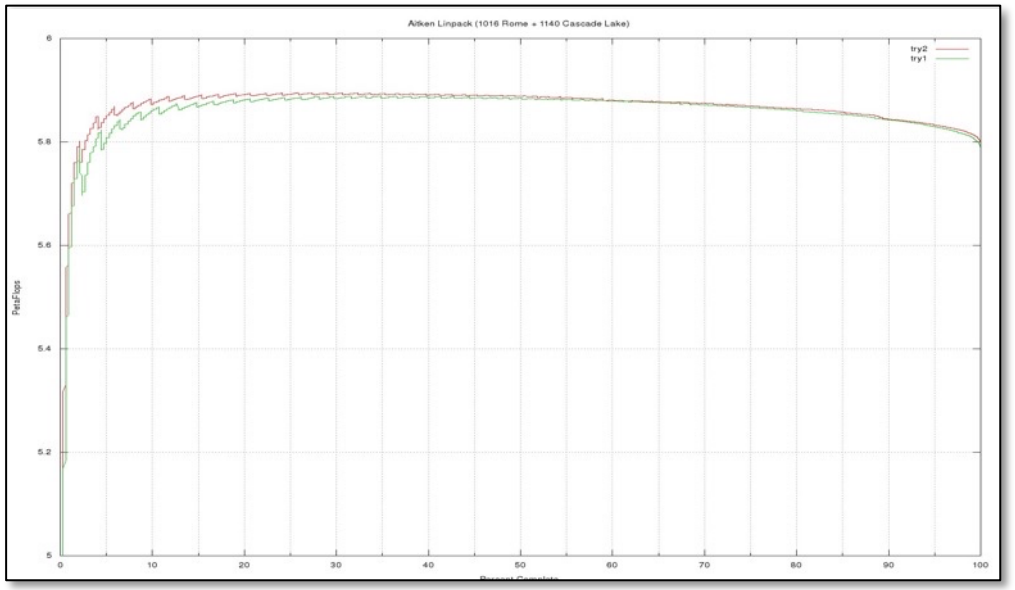


Chart showing two successful LINPACK runs on Aitken. The last run was completed without errors and resulted in a 5.795-petaflop performance. The other run had a hardware error that slightly impacted the result. Each was completed in approximately 14 hours.

HECC Teams Lead NASA's Virtual SC20 Exhibit Effort

- HECC staff planned and produced NASA's successful virtual exhibit for SC20, the International Conference for High Performance Computing, Networking, Storage, and Analysis, held November 9–19.
- The NASA@SC20 website features 35 science and engineering projects enabled by HECC and NCCS supercomputers and supported by visualization, optimization, and machine learning experts. The projects represent researcher teams from three NASA locations, plus university and corporate collaborators.
- The HECC Tools team, in collaboration with the Publications and Media Team, conceived a strategy for bringing SC20 participants and the public to the NASA@SC20 virtual exhibit. Highlights this year include:
  - A revamped home page, featuring a welcome video and vibrant images invited visitors to link to each research project.
  - A special COVID-19 Research sidebar featured the agency's HPC support in the fight to understand the SARS-CoV-2 virus, and to develop treatments and vaccines.
  - Researchers' headshots on each project page promoted a connection with website visitors, in lieu of in-person introductions.
  - Digital swag replaced the always sought-after luggage tags, NASA stickers, and other handouts offered each year. The ringtones, desktop and mobile wallpapers, and virtual backgrounds proved highly popular—along with a HECC-produced Music from Mars video.
  - A carefully curated social media campaign to draw the public to the virtual exhibit via Twitter and Facebook.

IMPACT: Participating in the annual supercomputing conference provides a public platform to showcase NASA science and engineering projects supported by the agency's high-performance computing (HPC) resources, as well as NASA's latest advances in HPC technologies.

The NASA@SC20 website features more than 70 images and 30 videos from 35 research projects, with a page for each project to explain the research details, results, and impact. New this year are a welcome video and "digital swag" giveaways, including ringtones based on Mars weather forecast simulations run on the Pleaides supercomputer. *John Hardman, NASA Ames*

Papers

- "**A Synthesis of Upper Ocean Geostrophic Kinetic Energy Spectra from a Global Submesoscale Permitting Simulation**," H. Khatri, et al., Earth and Space Science Open Archive, November 3, 2020. * https://search.proquest.com/docview/2457135078
- "**Pore-Resolved Simulations of Porous Media Combustion with Conjugate Heat Transfer**," J. Ferguson, S. Sobhani, M. Ihme, Proceedings of the Combustion Institute, published online November 10, 2020. * https://www.sciencedirect.com/science/article/abs/pii/S154074892030119X
- "**REACTER: A Heuristic Method for Reactive Molecular Dynamics**," J. Gissinger, B. Jensen, K. Wise, Macromolecules (American Chemical Society), vol. 53, issue 22, November 11, 2020. * https://pubs.acs.org/doi/abs/10.1021/acs.macromol.0c02012
- "**Deep Convection-Driven Vortex Formation on Jupiter and Saturn**," R. Yadav, M. Heimpel, J. Bloxham, Science Advances, vol. 6, no. 46, November 13, 2020. * https://advances.sciencemag.org/content/6/46/eabb9298.abstract
- "**Binary Planetesimal Formation from Gravitationally Collapsing Pebble Clouds**," D. Vesvorny, et al., arXiv:2011.07042 [astro-ph.EP], November 13, 2020. * https://arxiv.org/abs/2011.07042
- "**Igniting Weak Interactions in Neutron-Star Post-Merger Accretion Disks**," S. De, D. Siegel, arXiv:2011.07176 [astro-ph.HE], November 14, 2020. * https://arxiv.org/abs/2011.07176

** HECC provided supercomputing resources and services in support of this work*

Papers (cont.)

- "**TESS Science Processing Operations Center FFI Target List Products**," D. Caldwell, et al., Research Notes of the American Astronomical Society, vol. 4, no. 11, November 17, 2020. *
  https://iopscience.iop.org/article/10.3847/2515-5172/abc9b3/meta
- "**Including Beyond-Linear Halo Bias in Halo Models**," A. Mead, L. Verde, arXiv:2011.08858 [astro-ph.CO], November 17, 2020. *
  https://arxiv.org/abs/2011.08858
- "**Black Hole-Neutron Star Coalescence: Effects of the Neutron Star Spin on Jet Launching and Dynamical Ejecta Mass**," M. Ruiz, et al., arXiv:2011.08863 [astro-ph.HE], November 17, 2020. *
  https://arxiv.org/abs/2011.08863
- **2020 Supercomputing Conference**, virtual event, November 17–20, 2020.
  - "**Aeroelasticity of Electric Vertical Take-off and Landing Air Taxis**," G. Guruswamy. *
    https://www.nas.nasa.gov/SC20/demos/demo1.html
  - "**Generating Aerodynamic Databases for NASA's X-57 Maxwell Aircraft**," J. Duensing, C. Kiris. *
    https://www.nas.nasa.gov/SC20/demos/demo2.html
  - "**CFD Support for Enabling Commercial Supersonic Flight**," J. Jensen, M. Aftosmis, M. Nemec, C. Kiris. *
    https://www.nas.nasa.gov/SC20/demos/demo3.html
  - "**Developing Best Practices for Transonic-Truss Braced Wing Aircraft Simulation**," D. Maldonado, J. Housman, J. Duensing, C. Kiris. *
    https://www.nas.nasa.gov/SC20/demos/demo4.html
  - "**Predicting Corner-Flow Separation in a Wing-Body Juncture using Scale Resolving Simulations**," A. Ghate, G.-D. Sitch, J. Housman, G. Kenway, C. Kiris. *
    https://www.nas.nasa.gov/SC20/demos/demo5.html

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Papers (cont.)

- **2020 Supercomputing Conference** (cont.)
  - "**Predicting Jet Noise for Full-Scale Low-Boom Aircraft**," G.-D. Stich, J. Housman, A. Ghate, C. Kiris. * https://www.nas.nasa.gov/SC20/demos/demo6.html
  - "**CFD Simulations of Complex Multirotor Test Systems in a Wind Tunnel**," J. Ahmad, W. Chan, S. Conley, C. Russel. * https://www.nas.nasa.gov/SC20/demos/demo7.html
  - "**Designing Active Flow Control Actuators for High-Lift Wing Configurations**," V. Vasta, L. Melton, R. Ferris, J. Lin, D. Lockard. * https://www.nas.nasa.gov/SC20/demos/demo8.html
  - "**Developing Aerodynamic Databases for Artemis' Booster Separation Event**," J. Meeroff, S. Rogers, A. Burkhead, D. Schauerhamer. * https://www.nas.nasa.gov/SC20/demos/demo9.html
  - "**Predicting Orion Supersonic Ascent Abort Vibrations to Keep Astronauts Safe**," F. Cadieux, M. Barad, J. Jensen, C. Kiris. * https://www.nas.nasa.gov/SC20/demos/demo10.html
  - "**High-Fidelity Multiphase Simulations of the KSC Launch Environment**," M. Barad, J. Angel, E. Sozer, J. Jensen, C. Kiris. * https://www.nas.nasa.gov/SC20/demos/demo11.html
  - "**Modeling the Impact of Martian Dust on Atmospheric Entry Vehicles**," E. Ching, M. Ihme. * https://www.nas.nasa.gov/SC20/demos/demo12.html
  - "**Simulations of Giant Cold Fronts in Clusters of Galaxies**," J. ZuHone, S. Walker, J. Sanders, A. Fabrian. * https://www.nas.nasa.gov/SC20/demos/demo13.html
  - "**HECC: Meeting Today's Needs, Planning for the Future**," W. Thigpen. https://www.nas.nasa.gov/SC20/demos/demo14.html
  - "**Seeking Earth's Closest Cousins: TESS's All-Sky Survey**," J. Jenkins. * https://www.nas.nasa.gov/SC20/demos/demo15.html

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Papers (cont.)

- **2020 Supercomputing Conference** (cont.)
  - "**Imaging the Solar Interior: Emerging Active Regions**," J. Stephan, A. Kosovichev. * https://www.nas.nasa.gov/SC20/demos/demo16.html
  - "**New Modeling Tools Help Explore the Interior of the Sun**," A. Stejko, A. Kosovichev. * https://www.nas.nasa.gov/SC20/demos/demo17.html
  - "**3D Realistic Modeling of Rotating Stars**," Irina Kitiashvili, A. Wray. * https://www.nas.nasa.gov/SC20/demos/demo18.html
  - "**Modeling Observations of NASA Heliophysics Missions from Realistic Simulations of the Sun**," V. Sadykov, I. Kitiashvili, A. Kosovichev, A. Wray. * https://www.nas.nasa.gov/SC20/demos/demo19.html
  - "**Predicted Expansion of the South Atlantic Anomaly in the Next Five Years**," W. Kuang, T. Sabaka, A. Tangborn, C. Yi. * https://www.nas.nasa.gov/SC20/demos/demo20.html
  - "**Understanding How Violent Cosmic Events Create Heavy Elements**," D. Siegel, B. Metzger. * https://www.nas.nasa.gov/SC20/demos/demo28.html
  - "**SARS-CoV-2 Spike Protein: Unlocking the Pick that Picks Our Cells**," O. Bastidas, M. Peters. * https://www.nas.nasa.gov/SC20/demos/demo29.html
  - "**Drug Repurposing for COVID-19 with 3D-Aware Machine Learning**," S. Axelrod, R. Gomez-Bombarelli. * https://www.nas.nasa.gov/SC20/demos/demo30.html
  - "**Gene Hub Analysis to Identify Host Response to COVID-19**," R. Meller, D. Taylor, C. Mason, A. Saravia-Bulter, A. Behesti, J. Schisler. * https://www.nas.nasa.gov/SC20/demos/demo32.html

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Papers (cont.)

- **2020 Supercomputing Conference** (cont.)
  - "**Examining the Dynamics of the 'Dark Genome' in Response to SARS-CoV-2 Infection**," F. Enguita, A. Behesti, G. Karebach, P. Robinson, A. Saravia-Butler, C. Mason. * https://www.nas.nasa.gov/SC20/demos/demo33.html
  - "**Identifying the Genetic Ancestry of COVID-19 Patients from New York City**," A. Conley, A. Saravia-Butler, C. Mason, S. Nagar, R. Meller. * https://www.nas.nasa.gov/SC20/demos/demo34.html
  - "**NAS Data Portal: Distributing Large, High-Volume Computational Datasets**," S. Ranjan, R. Spaulding, G. Deardorff. https://www.nas.nasa.gov/SC20/demos/demo35.html
  - "**Application Support for Effective Use of NASA HPC Resources**," R. Hood. H. Jin. https://www.nas.nasa.gov/SC20/demos/demo36.html
- "**TOI-519 b: A Short-Period Substellar Object Around an M Dwarf Validated Using Multicolour Photometry and Phase Curve Analysis**," H. Parviainen, et al., arXiv:2011.11458 [astro-ph.EP], November 23, 2020. * https://arxiv.org/abs/2011.11458
- "**Observational Constraints on the Response of High-Latitude Northern Forests to Warming**," J. Liu, et al., American Geophysical Union: Advances, vol.1, issue 4, November 24, 2020. * https://agupubs.onlinelibrary.wiley.com/doi/full/10.1029/2020AV000228

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News and Events

- **NASA Research Exhibit to Highlight Science and Engineering Advances at the Virtual SC20 Supercomputing Conference**, *NASA Goddard*, November 16, 2020—From assessing COVID-19's global impacts to helping NASA return humans to the Moon to searching the cosmos for new exoplanets, researchers from across NASA, with university and industry partners, will highlight their latest advances, enabled by the agency's supercomputers, in the NASA research exhibit at SC20—the International Conference for High Performance Computing, Networking, Storage and Analysis. https://www.nasa.gov/press-release/goddard/2020/nasa-research-exhibit-to-highlight-science-and-engineering-advances-at-the-virtual
- **NASA Triples the Power of its Aitken Modular Supercomputer**, *NASA Advanced Supercomputing Division*, November 17, 2020—Engineers at the NAS facility expanded the petascale Aitken supercomputer, more than tripling the system's production capability to help solve NASA's most challenging problems. https://www.nas.nasa.gov/publications/articles/feature_aitken_expansion_fall_2020.html
  - **NASA Unveils New Research Progress for Human Mission to the Moon with Supercomputer Powered by Hewlett Packard Enterprise**, *Hewlett Packard Enterprise*, November 17, 2020. https://www.hpe.com/us/en/newsroom/press-release/2020/11/nasa-unveils-new-research-progress-for-human-mission-to-the-moon-with-supercomputer-powered-by-hewlett-packard-enterprise.html
  - **NASA Advances Human Mission to Moon with HPE-Powered Supercomputer**, *HPCwire*, November 17, 2020. https://www.hpcwire.com/off-the-wire/nasa-advances-human-mission-to-moon-with-hpe-powered-supercomputer/
  - **When Humans Return to the Moon in 2024, HPE Would Like Us to Remember: WE Built the Computer that Simmed This**, *The Register*, November 18, 2020. https://www.theregister.com/2020/11/18/hpe_aitken_upgrades/

News and Events (cont.)

- **Mars Calling: NASA Releases 'Out-of-this-World' Ringtone Made from Data on the Red Planet's Weather Patterns**, *Daily Mail*, November 17, 2020—Researchers from the UK have used NASA data to create new mobile phone ringtones that are quite literally out of this world. Dr. Domenico Vicinanza, of Anglia Ruskin University, and Dr. Genevieve Williams, of the University of Exeter, carried out the project to celebrate NASA's Pleiades supercomputer and its role in the successful Mars InSight mission.
  https://www.dailymail.co.uk/sciencetech/article-8958831/Mars-calling-NASA-releases-world-ringtone-using-data-Red-Planets-weather.html
  - **UK Researchers Dial into the Sound of Mars**, *Cambridge Network*, November 18, 2020.
    https://www.cambridgenetwork.co.uk/news/uk-researchers-dial-sound-mars
  - **UK Researchers Dial into the Sound of Mars**, *Anglia Ruskin University*, November 17, 2020.
    https://aru.ac.uk/news/uk-researchers-dial-in-to-the-sound-of-mars
- **NASA Supercomputers Visualize Quieter Supersonic Flight**, *NASA Ames*, November 17, 2020—NASA's X-59 Quiet SuperSonic Technology X-plane is designed to fly faster than the speed of sound without producing sonic booms. Researchers at the NASA Advanced Supercomputing (NAS) facility, in collaboration with Lockheed Martin, created a database of computational fluid dynamics simulations to verify the aircraft's supersonic performance. The X-59 simulations are performed on the NAS facility's Pleiades supercomputer.
  https://www.nasa.gov/image-feature/ames/nasa-supercomputers-visualize-quieter-supersonic-flight/

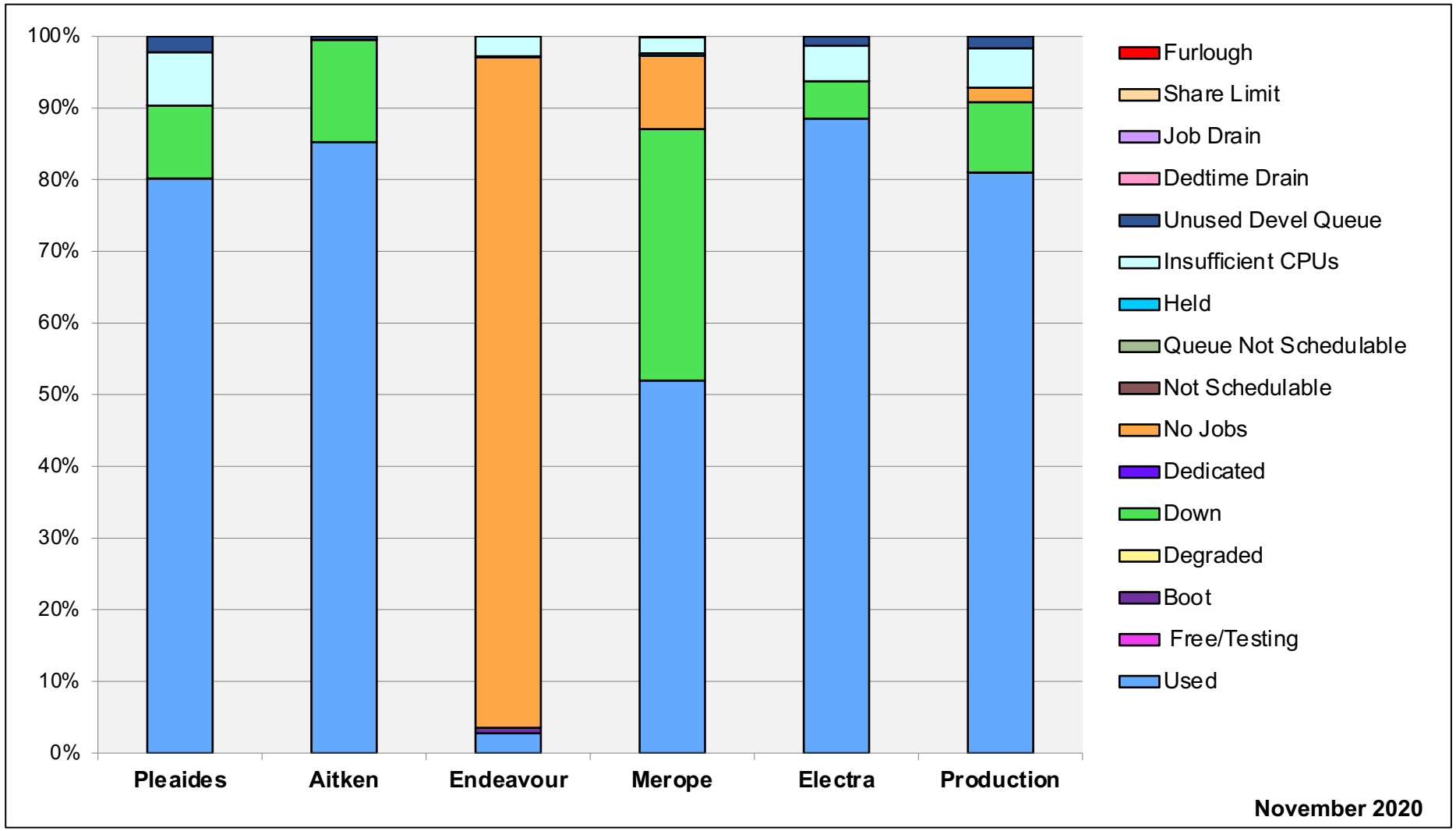
News and Events (cont.)

- **NASA Simulations Validate Orion Safety Models for Artemis Astronauts**, *NASA Ames*, November 18, 2020–As part of the Artemis program, NASA's Orion spacecraft will carry the first woman and next man to lunar orbit before they land on the Moon in 2024. An integral part of ensuring safe spaceflight is Orion's Launch Abort System (LAS). To better understand the effects of strong vibrations generated by the abort motor's high-speed exhaust plumes, a team at Ames produced high-fidelity simulations using NASA's Electra supercomputer.
  https://www.nasa.gov/image-feature/ames/orion-launch-abort-simulation
- **Simulating NASA's Rocket Launch for Artemis Moon Missions**, *NASA Ames*, November 19, 2020—As part of the Artemis program, NASA is preparing to test the integrated systems that will take crew on missions to the Moon, including a powerful new rocket that will launch crew and cargo to lunar orbit. There are many critical moments in a rocket's journey from the ground to orbit, but perhaps none more so than the moment of ignition from the launch pad. The LAVA team at NAS is creating complex simulations of this event using agency supercomputers.
  https://www.nasa.gov/image-feature/ames/launch-pad-simulations

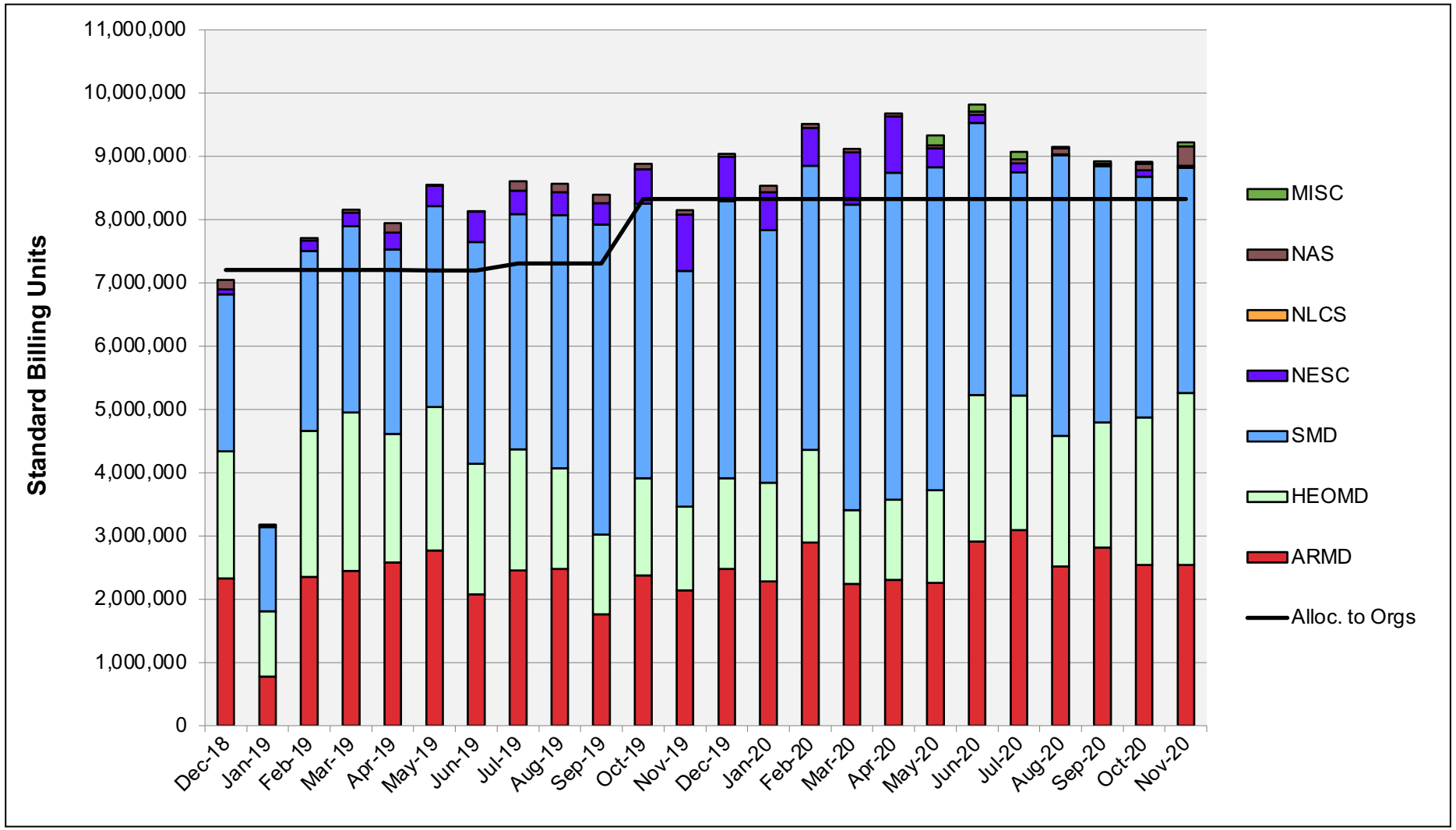
News and Events: Social Media

- **Coverage of NAS Stories**
  - NASA@SC20:
    - NASA Supercomputing: Facebook
      - Promotional Posts: Aeronautics, Human Space Flight, Earth Science, The Universe, NASA@SC exhibit
      - Giveaways: Backgrounds, Music from Mars, Wallpapers
    - NASA Supercomputing: Twitter collection
    - NASA Aeronautics: Facebook 51 likes, 7 shares; Twitter 24 retweets, 3 quote tweets, 117 likes
  - Artemis Launch Simulations:
    - NASA Supercomputing: Twitter 3 retweets, 1 quote tweet, 7 likes
    - NASA Ames: Facebook 106 likes, 12 shares; Twitter 27 retweets, 2 quote tweets, 226 likes
  - X-59 Supersonic X-plane simulations:
    - NASA Supercomputing: Facebook 194 users reached, 9 engagements, 6 likes; Twitter 1 retweet, 1 quote tweet, 2 likes
    - NASA Ames: Facebook 198 likes, 42 shares, 7 comments; Twitter 38 retweets, 3 quote tweets, 288 likes
    - NASA Aero: Facebook 4.7k likes, 22 comments, 218 shares; Twitter 22 retweets, 3 quote tweets, 144 likes
    - NASA Spinoff: Twitter 1 reply 1 retweet 10 likes
  - Orion Launch Abort Simulations:
    - NASA Supercomputing: Twitter 4 likes
    - Kathy Lueders (Associate Administrator, HEOMD): Twitter 28 retweets, 6 quote tweets, 294 likes

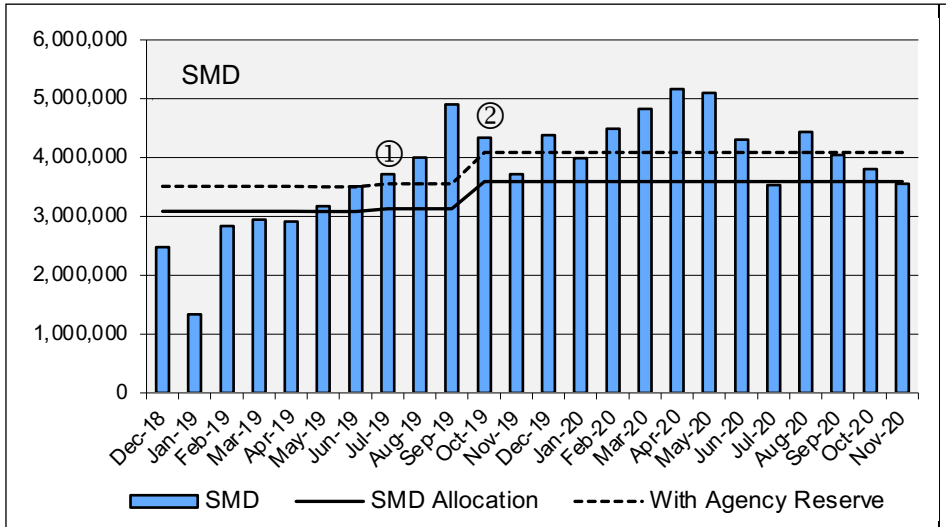
HECC Utilization

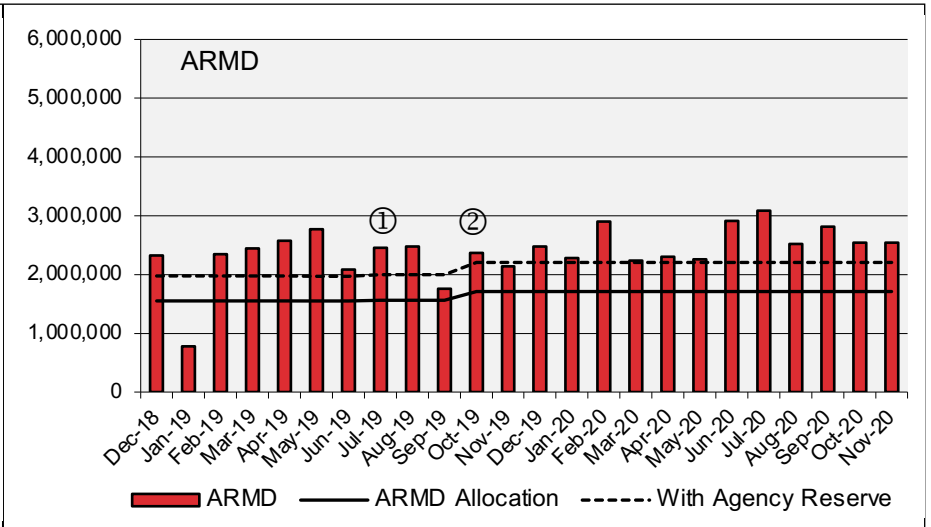


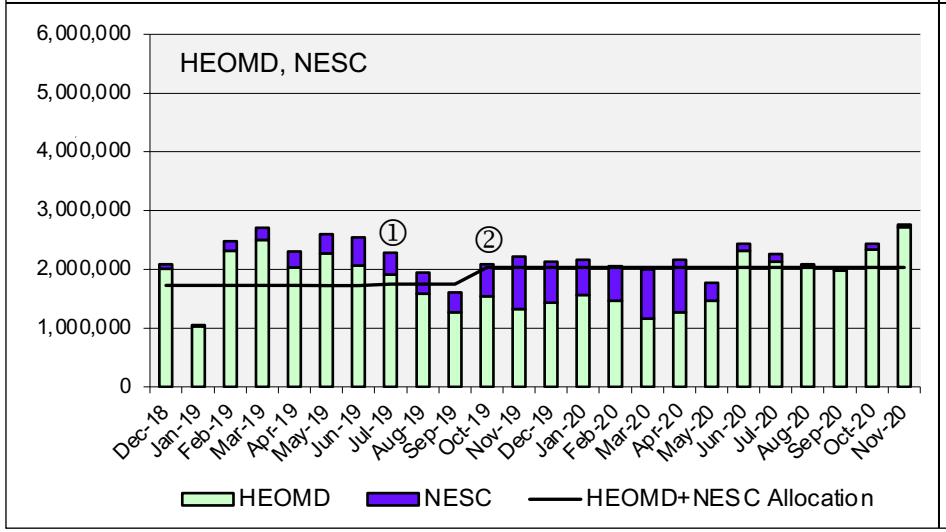
HECC Utilization Normalized to 30-Day Month



HECC Utilization Normalized to 30-Day Month



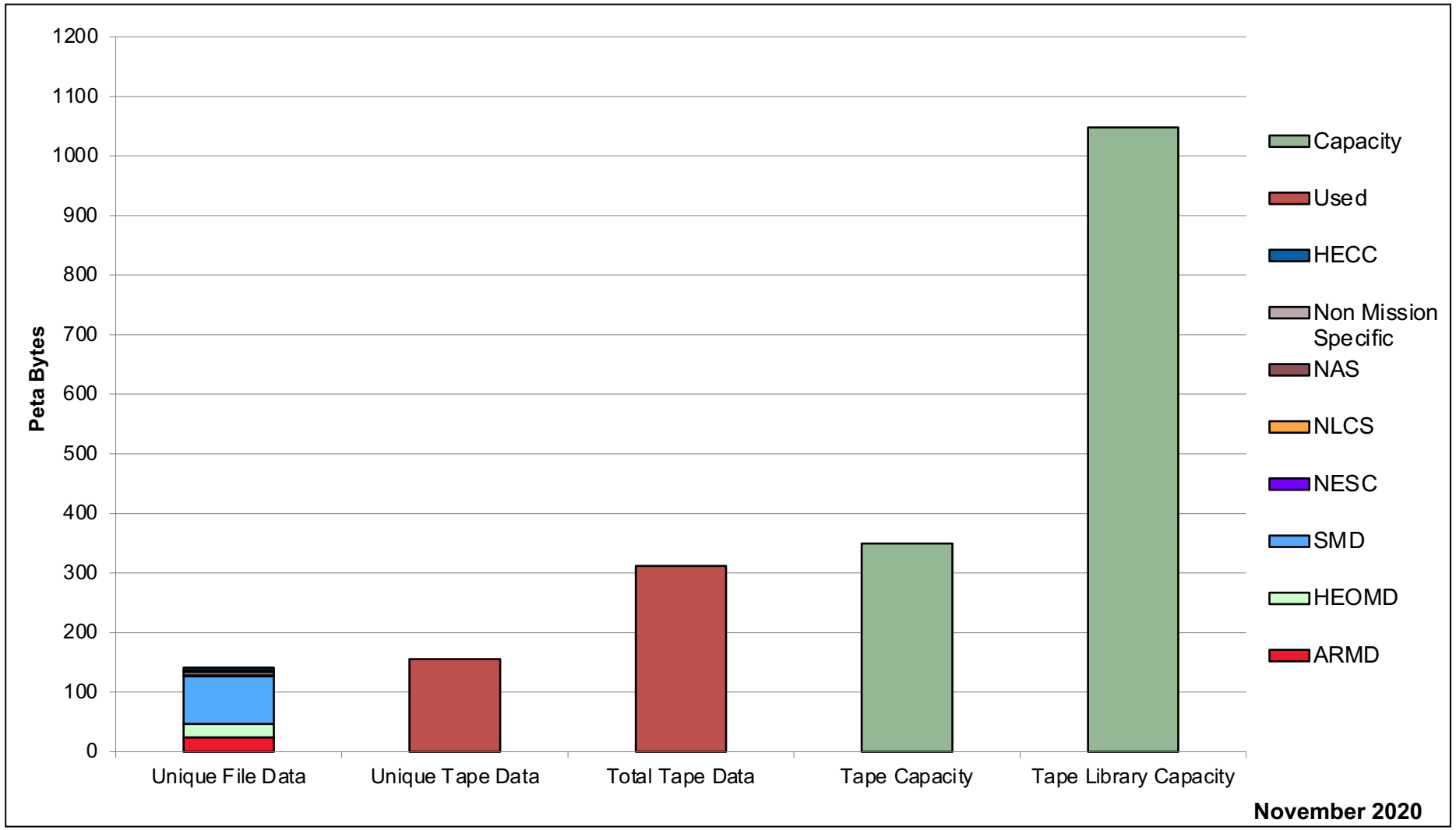




① Skylake Tesla GPU V100 Nodes installed

② 4 Cascade Lake E cells introduced into Aitken

Tape Archive Status



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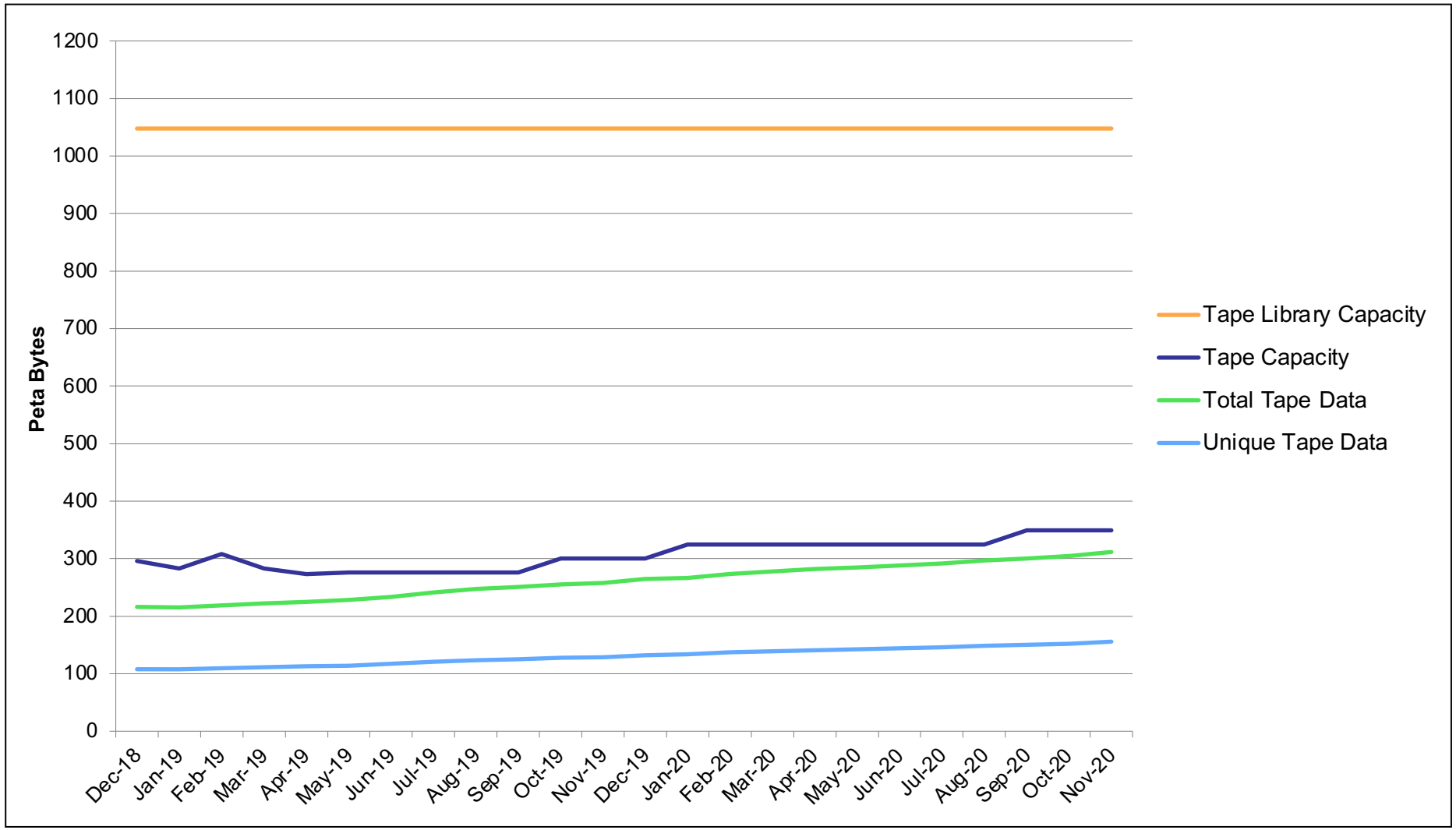
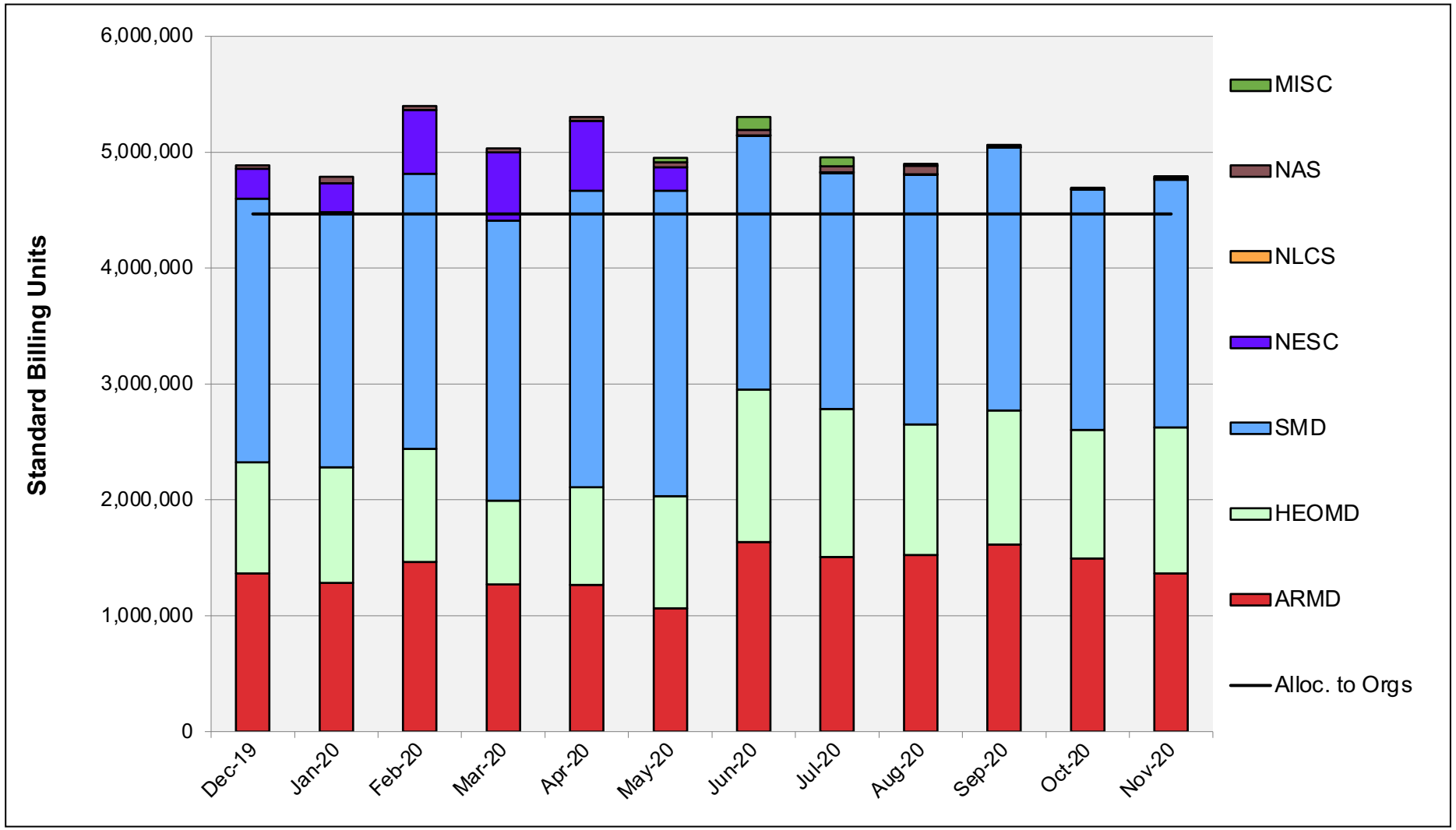
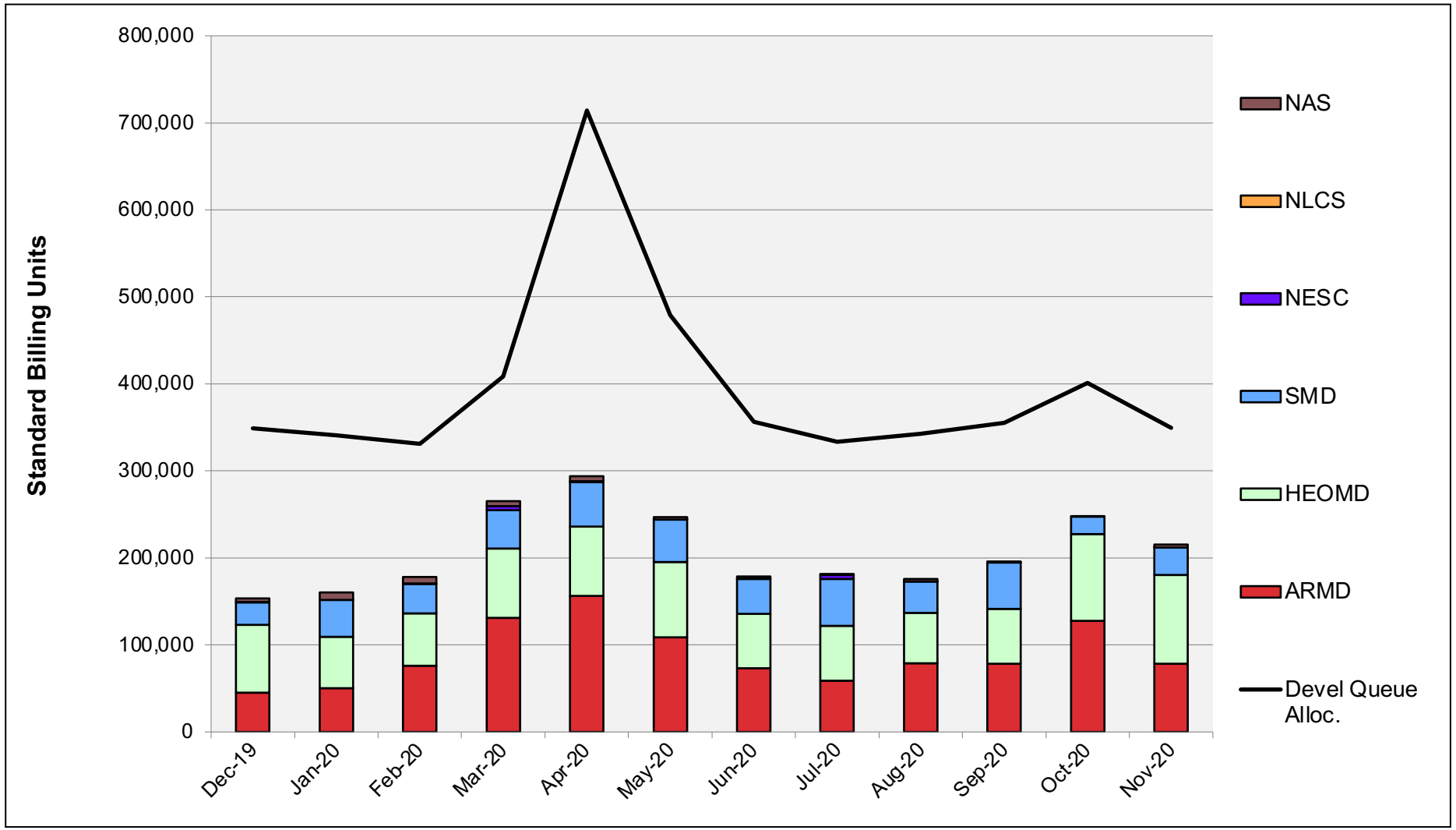


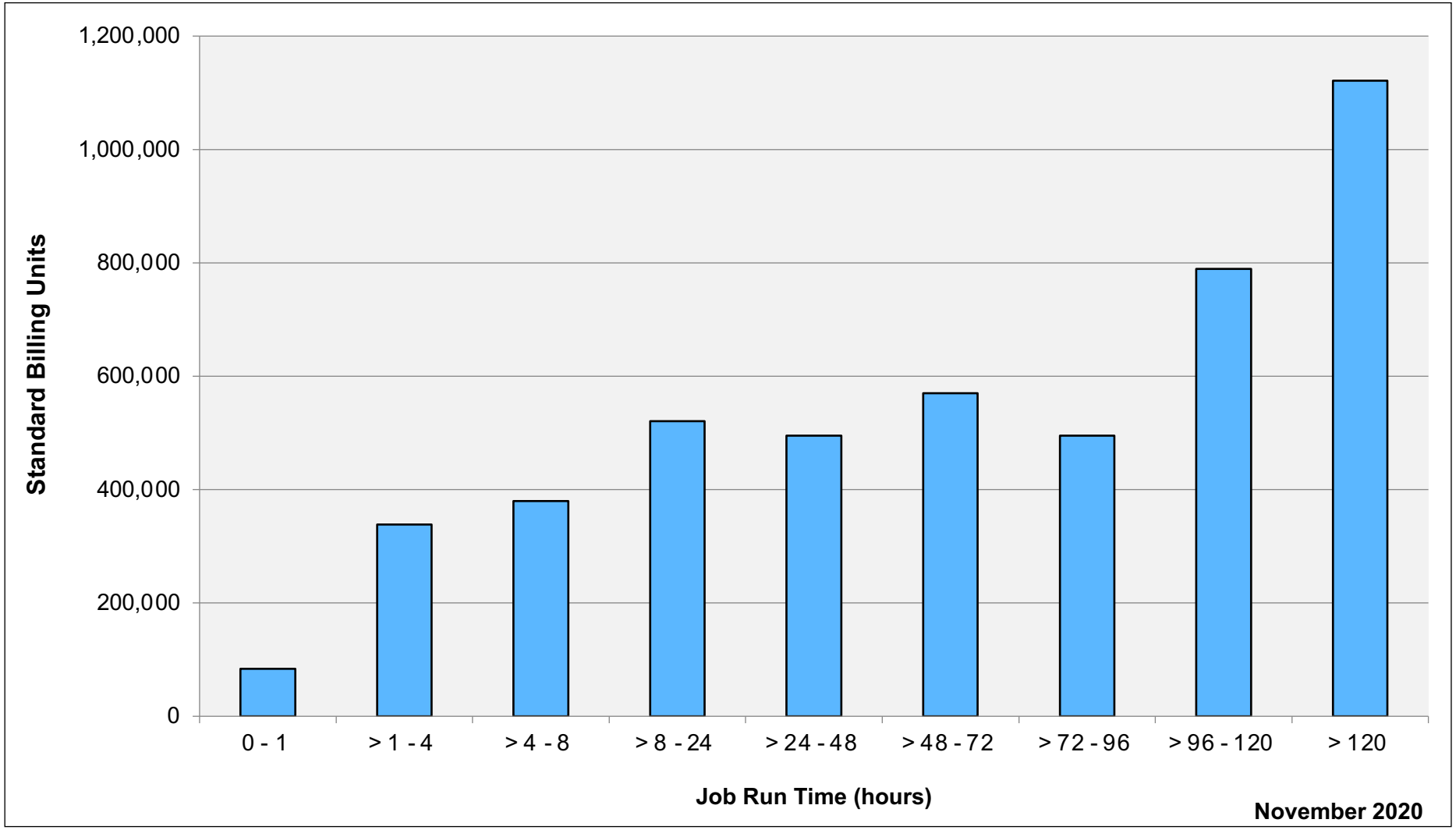
Pleiades: SBUs Reported, Normalized to 30-Day Month



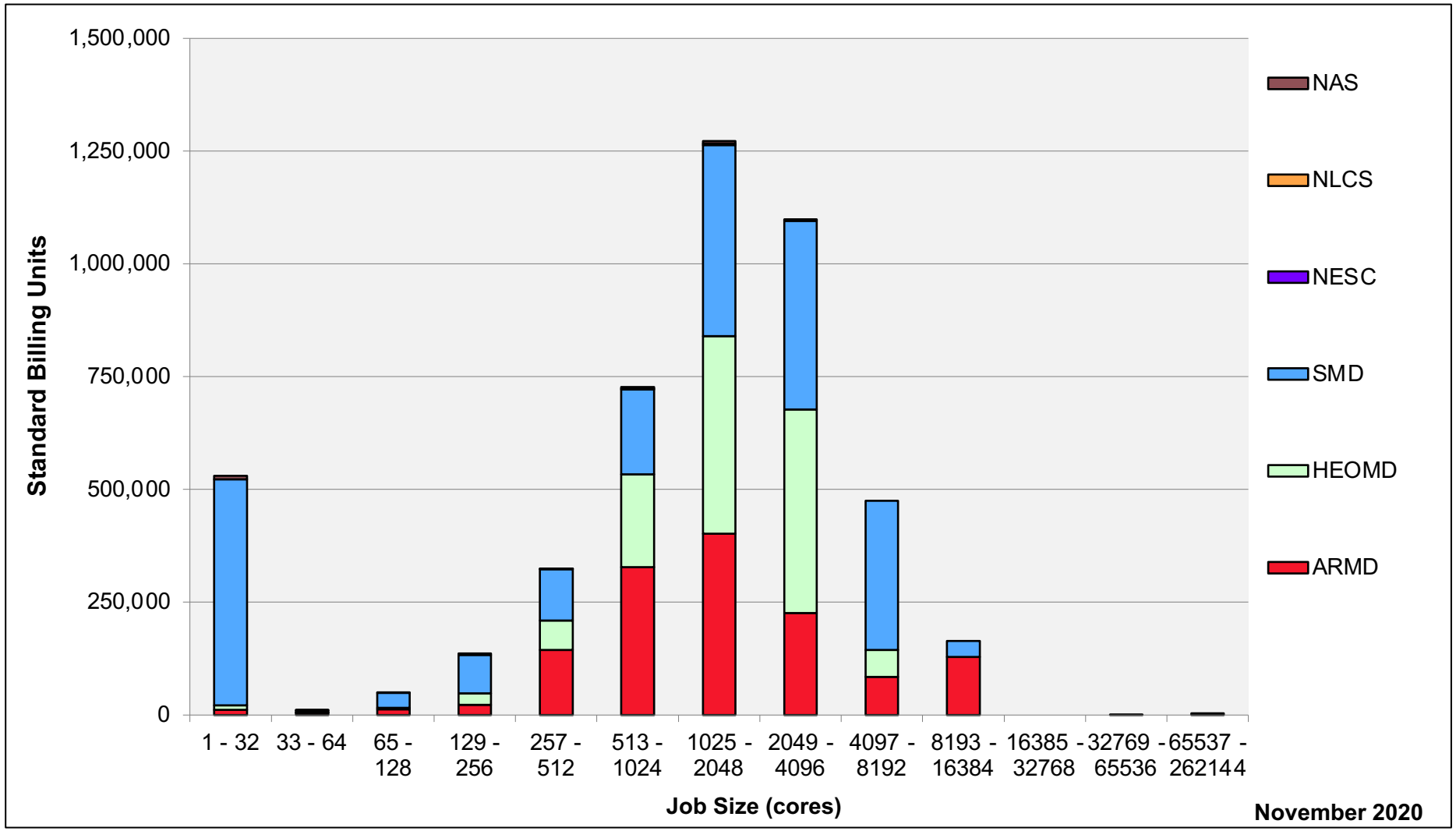
Pleiades: Devel Queue Utilization



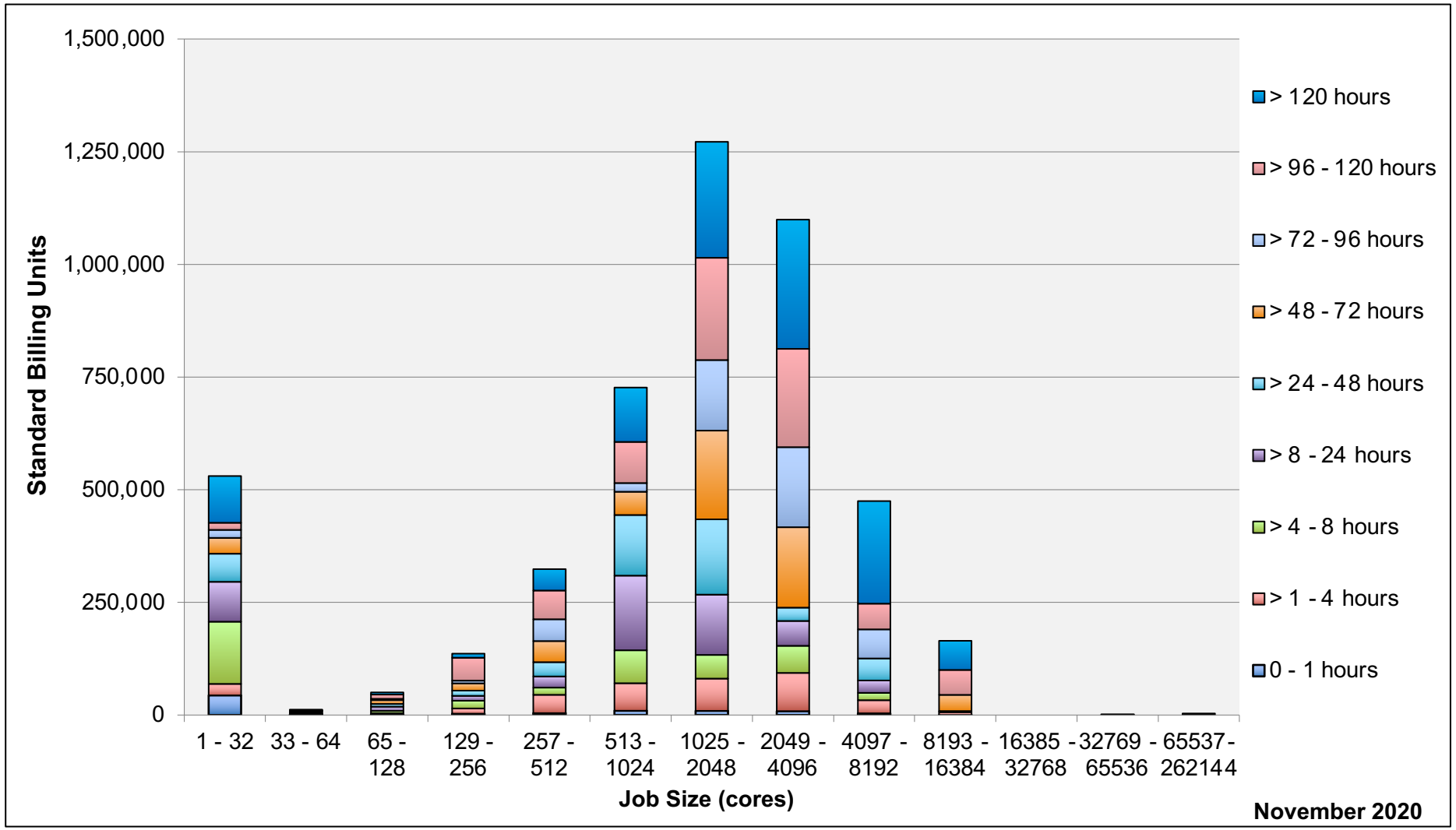
Pleiades: Monthly Utilization by Job Length



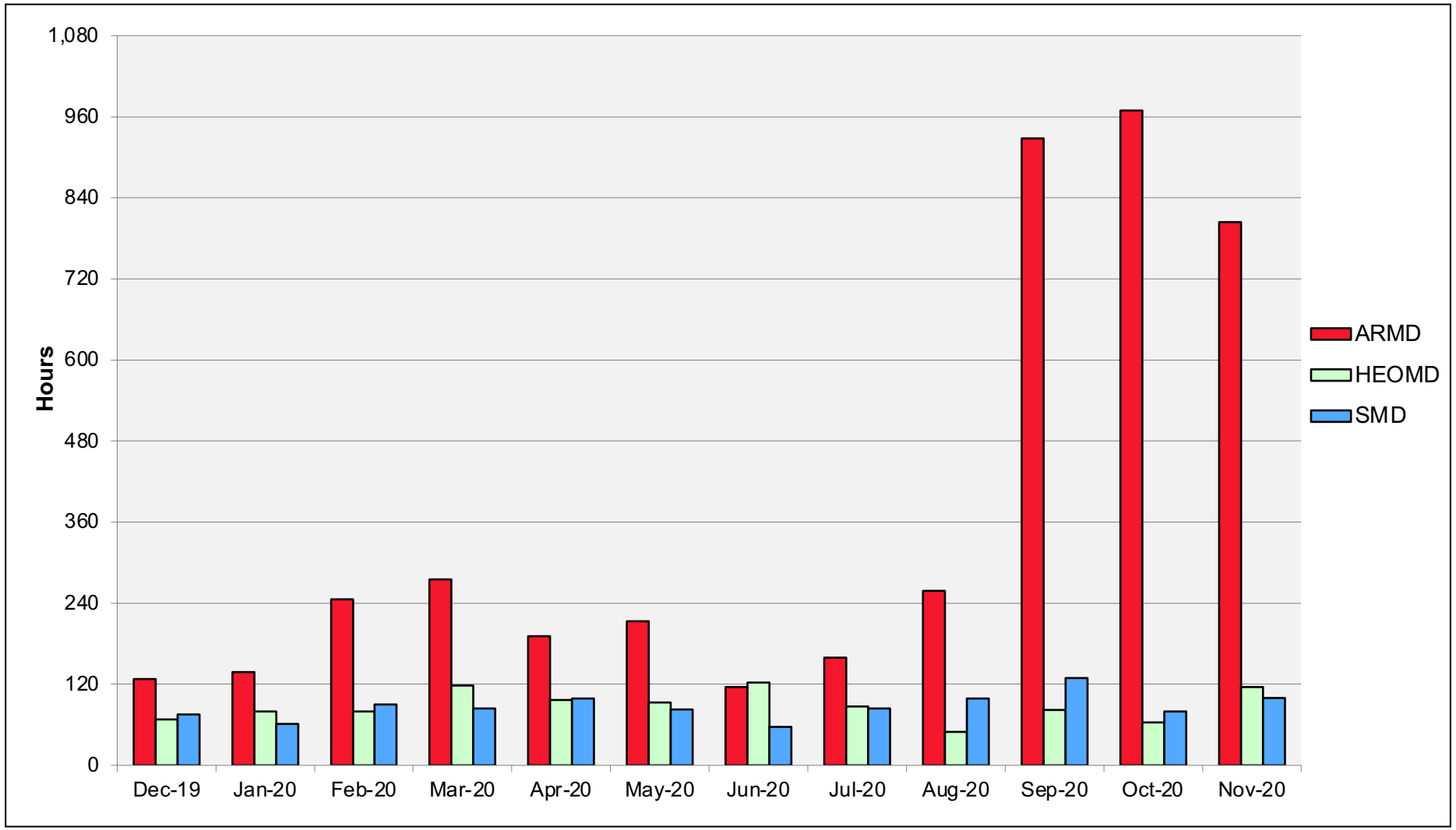
Pleiades: Monthly Utilization by Job Size



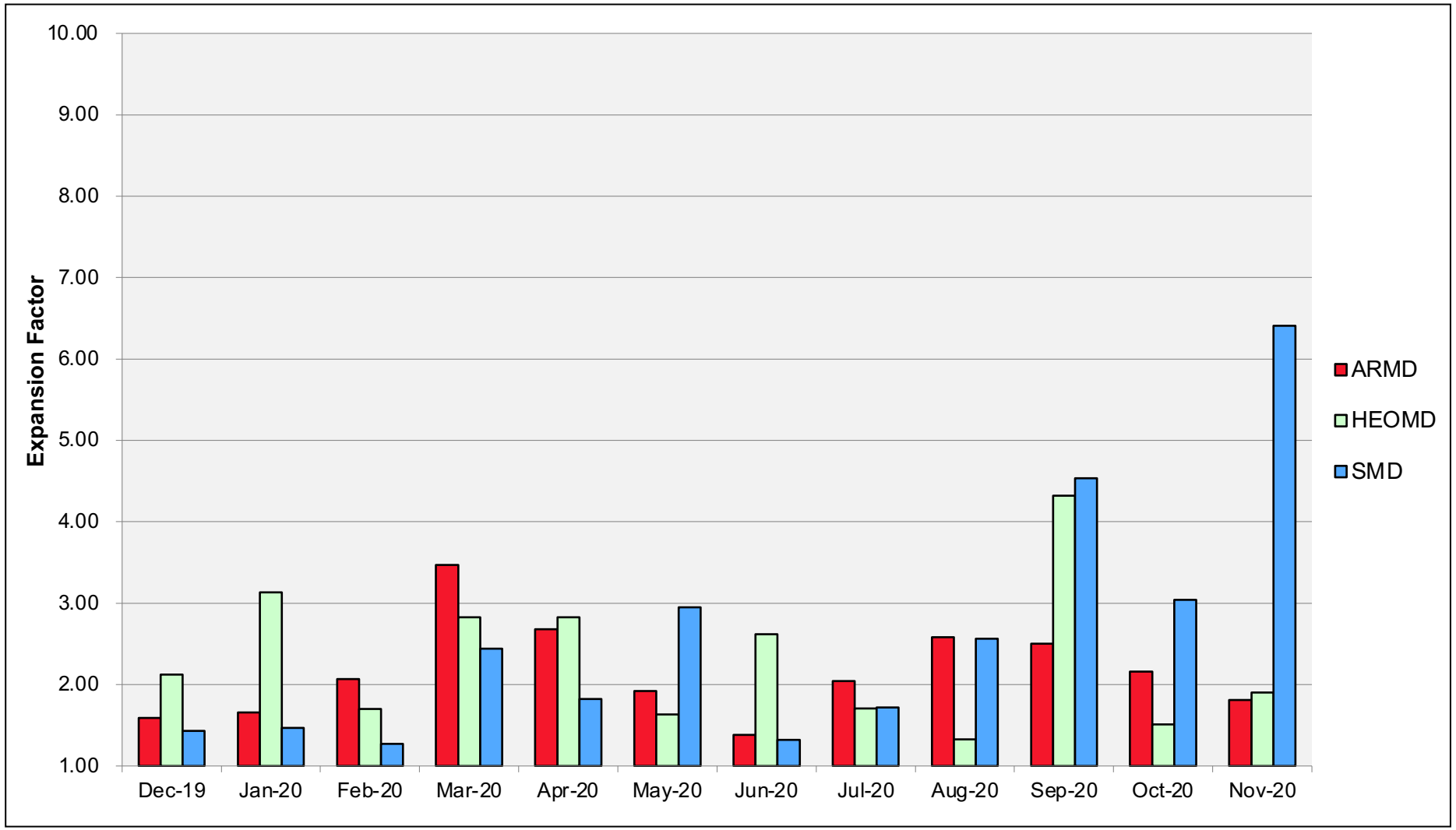
Pleiades: Monthly Utilization by Size and Length



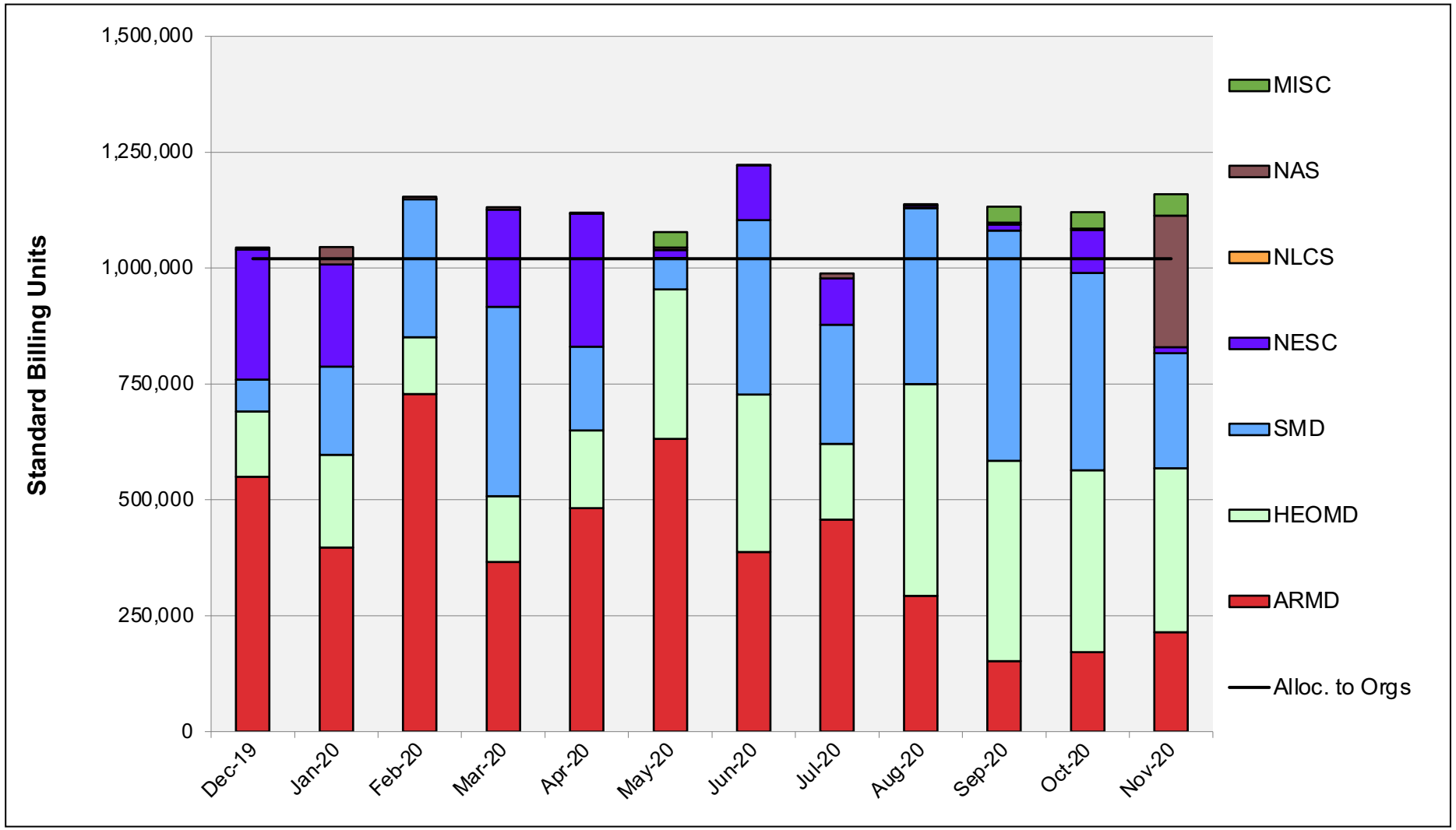
Pleiades: Average Time to Clear All Jobs



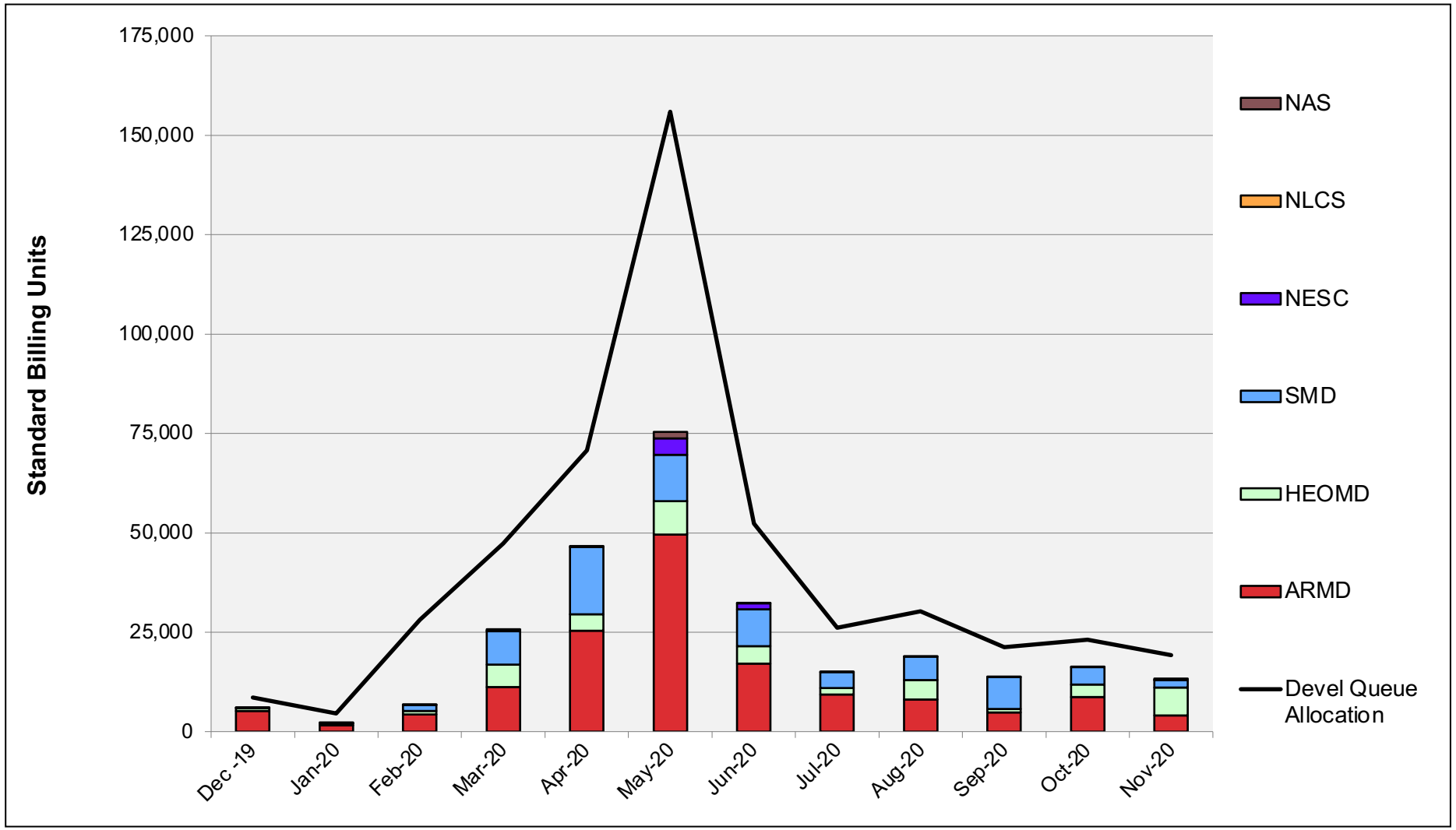
Pleiades: Average Expansion Factor



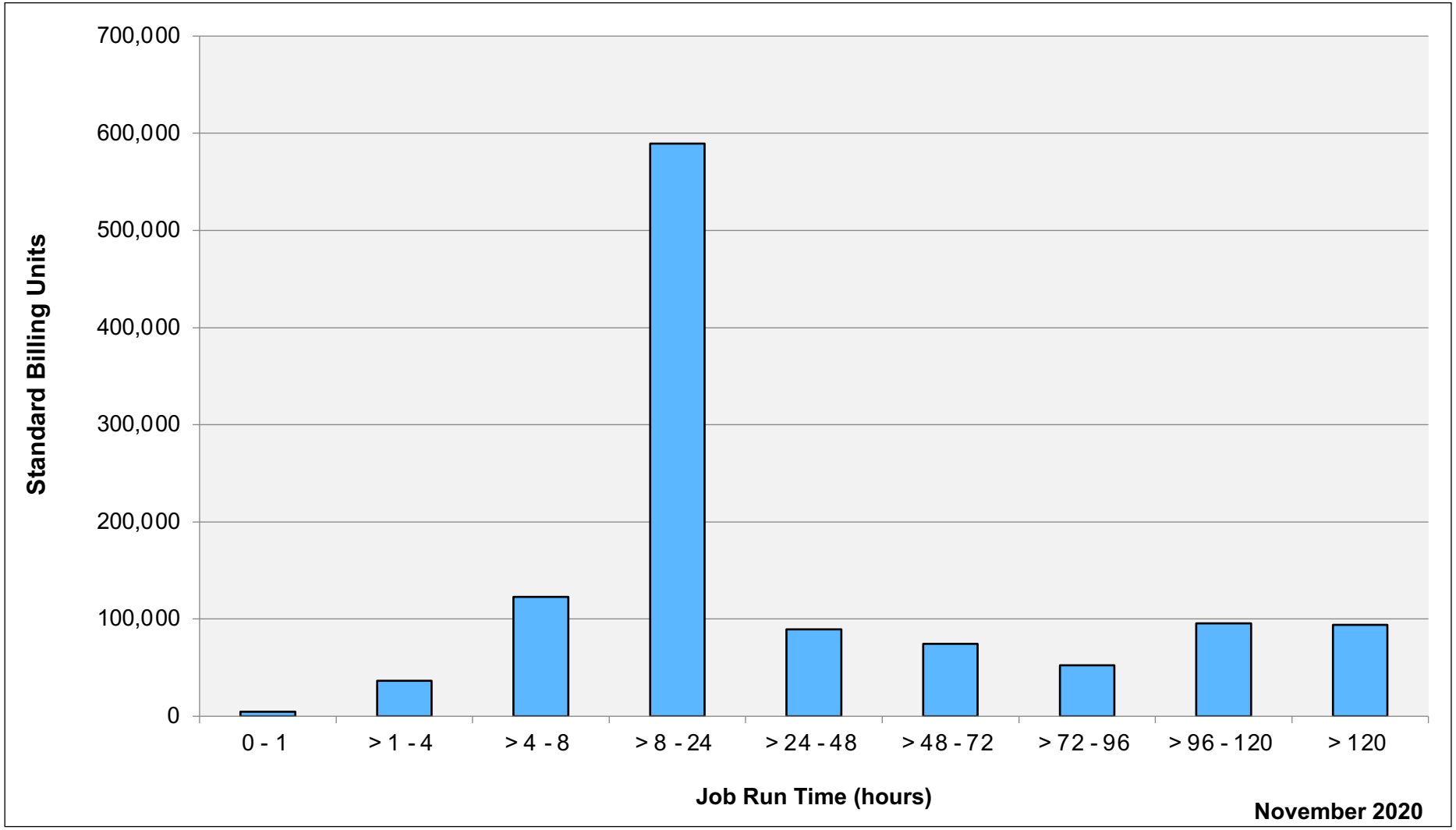
Aitken: SBUs Reported, Normalized to 30-Day Month



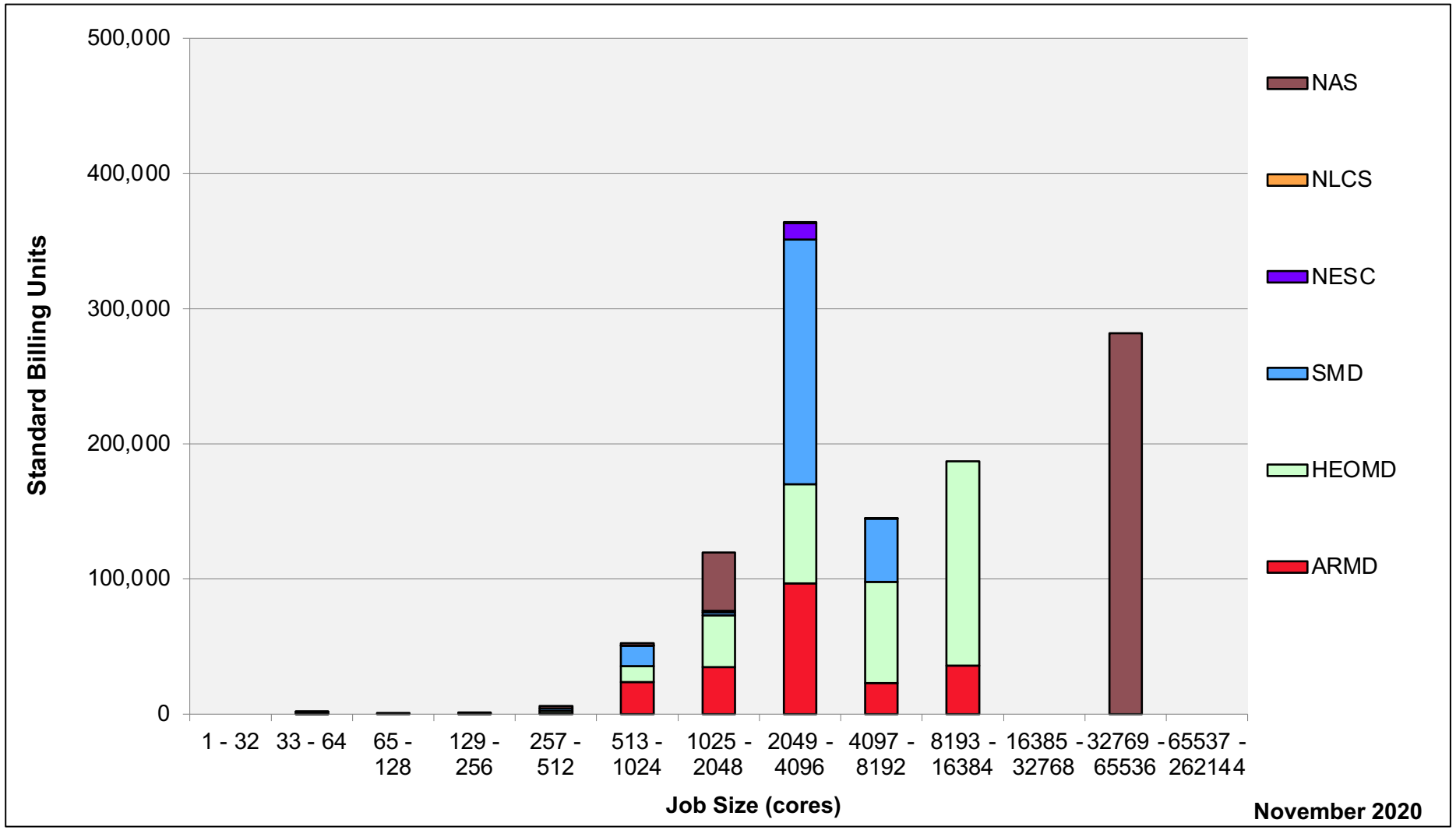
Aitken: Devel Queue Utilization



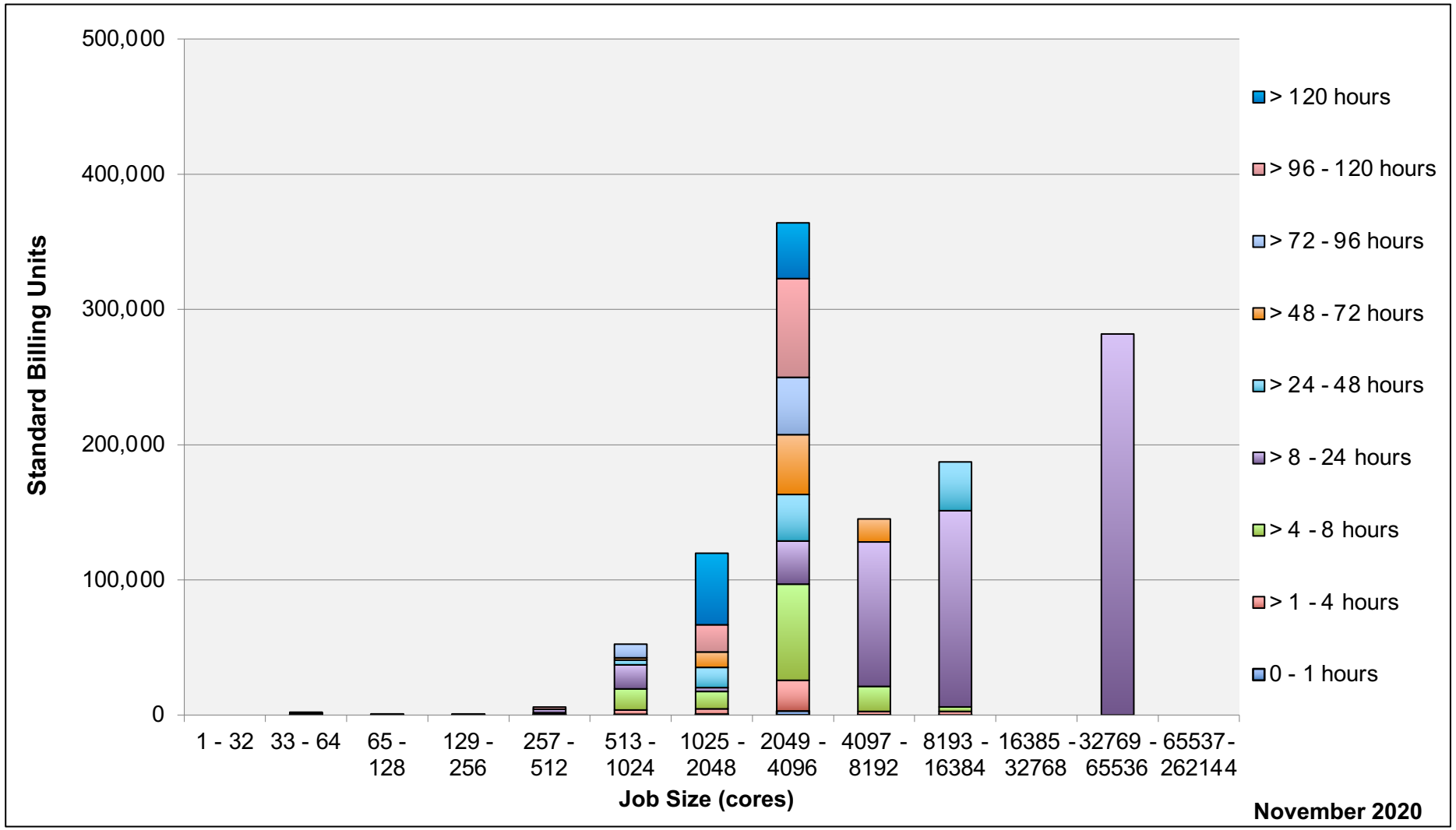
Aitken: Monthly Utilization by Job Length



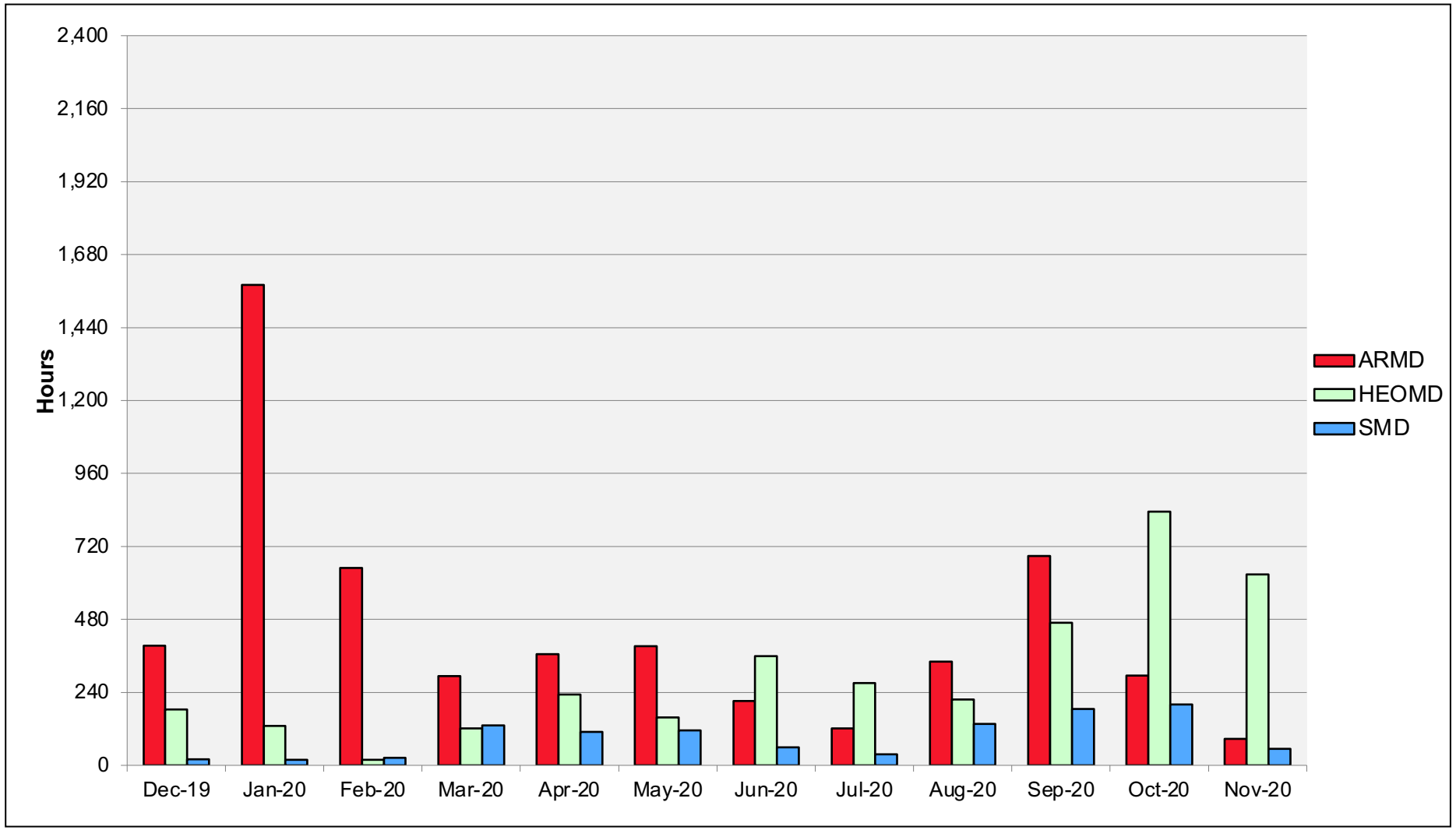
Aitken: Monthly Utilization by Job Size



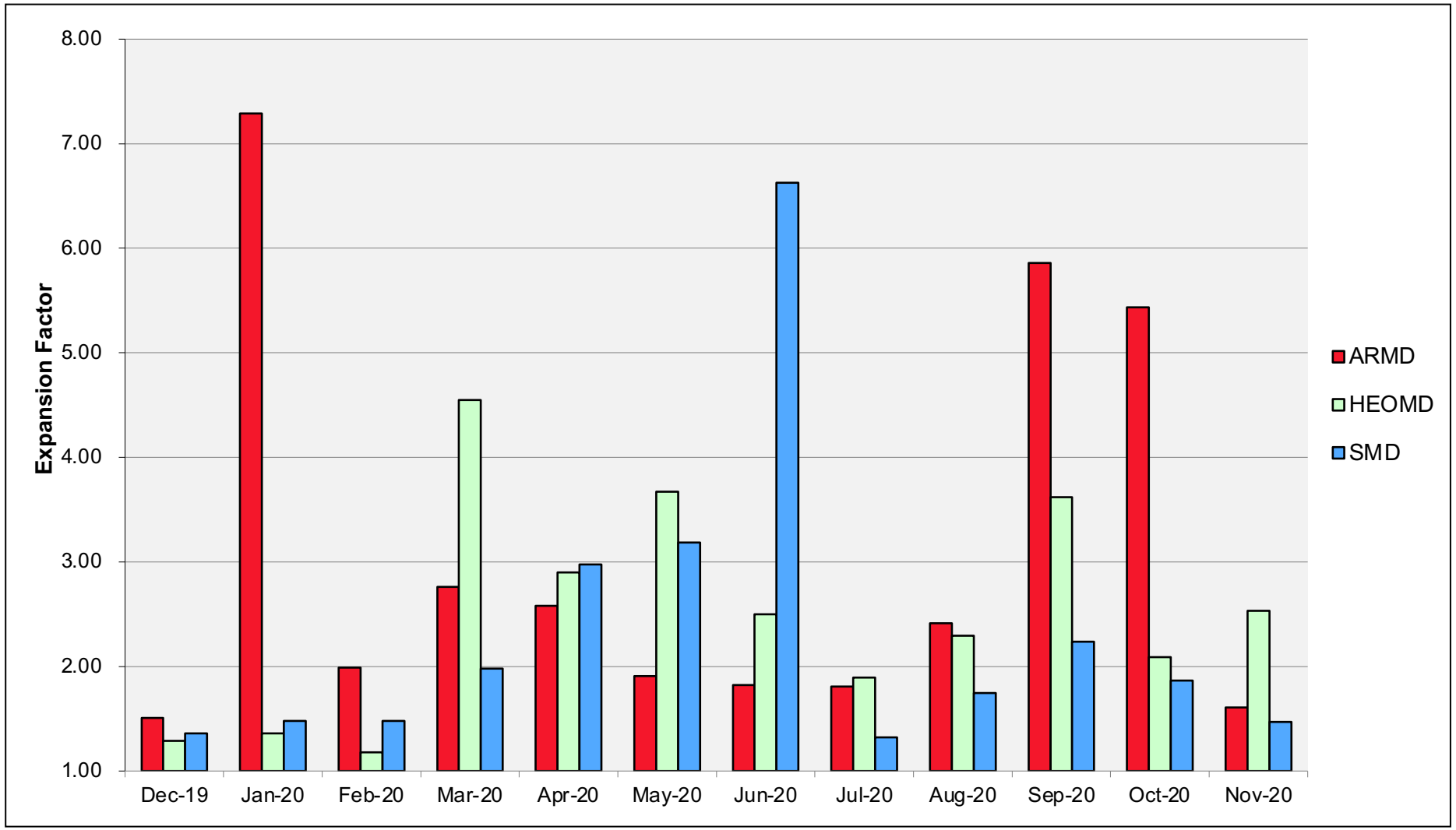
Aitken: Monthly Utilization by Size and Length



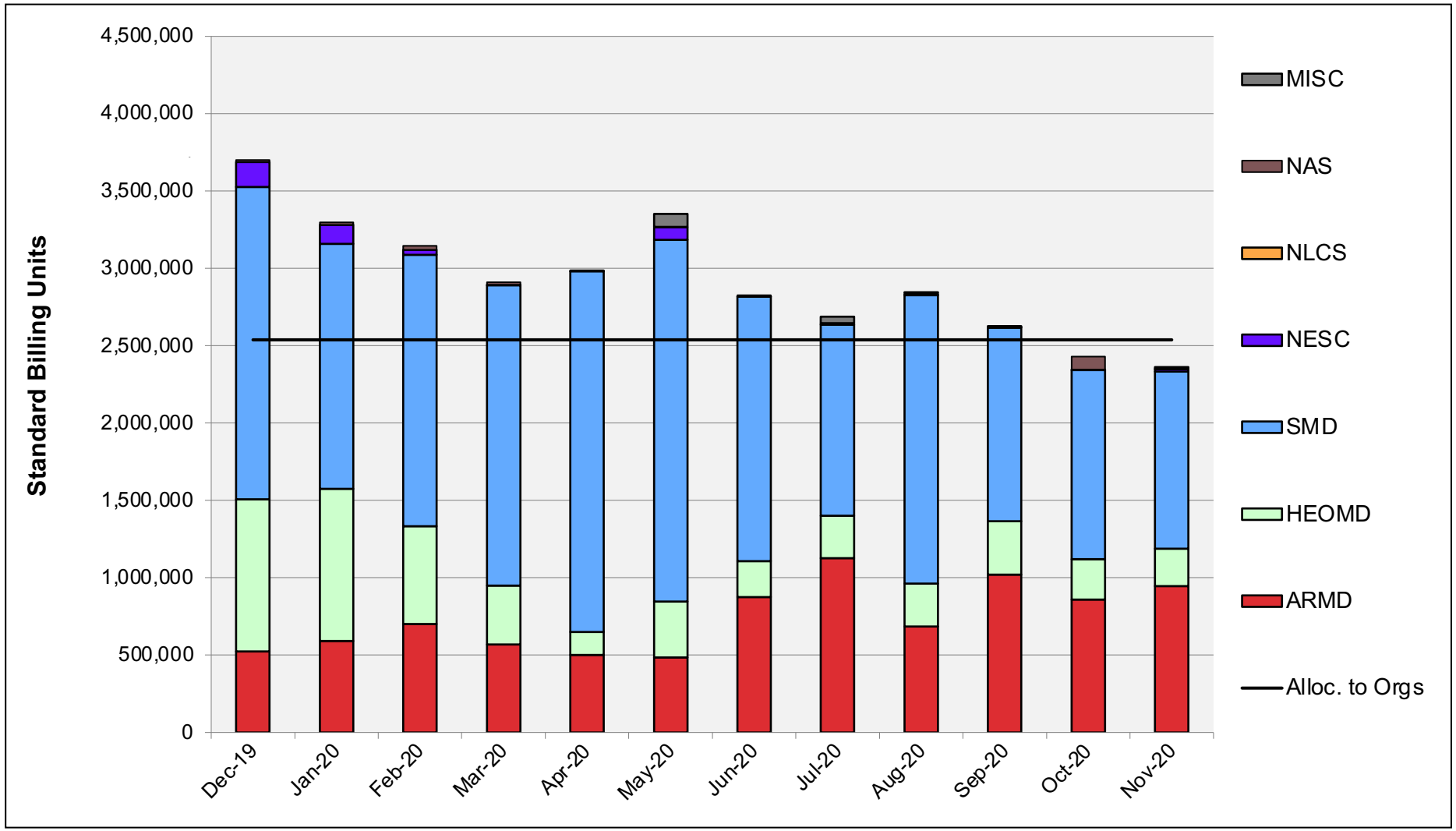
Aitken: Average Time to Clear All Jobs



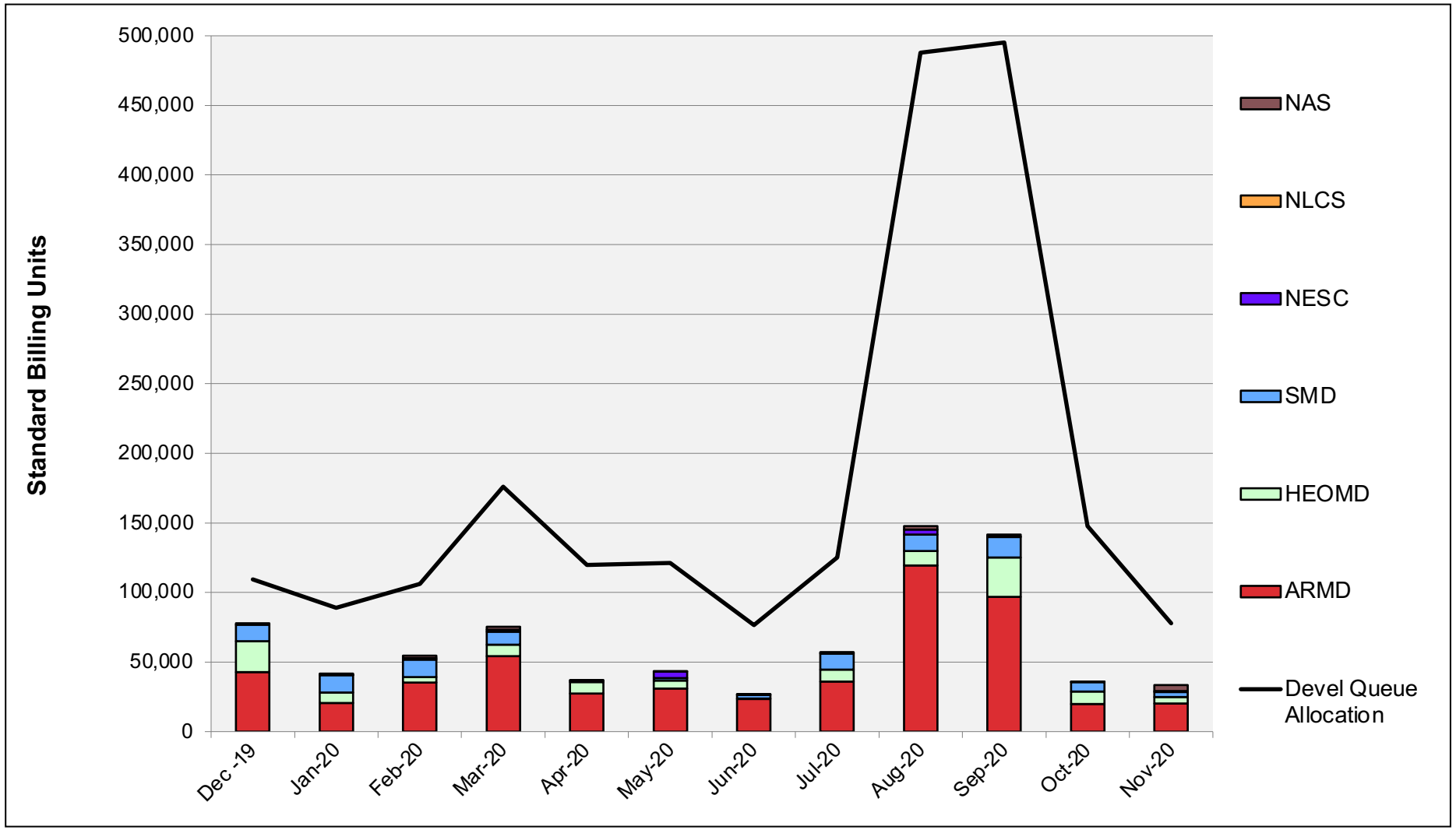
Aitken: Average Expansion Factor



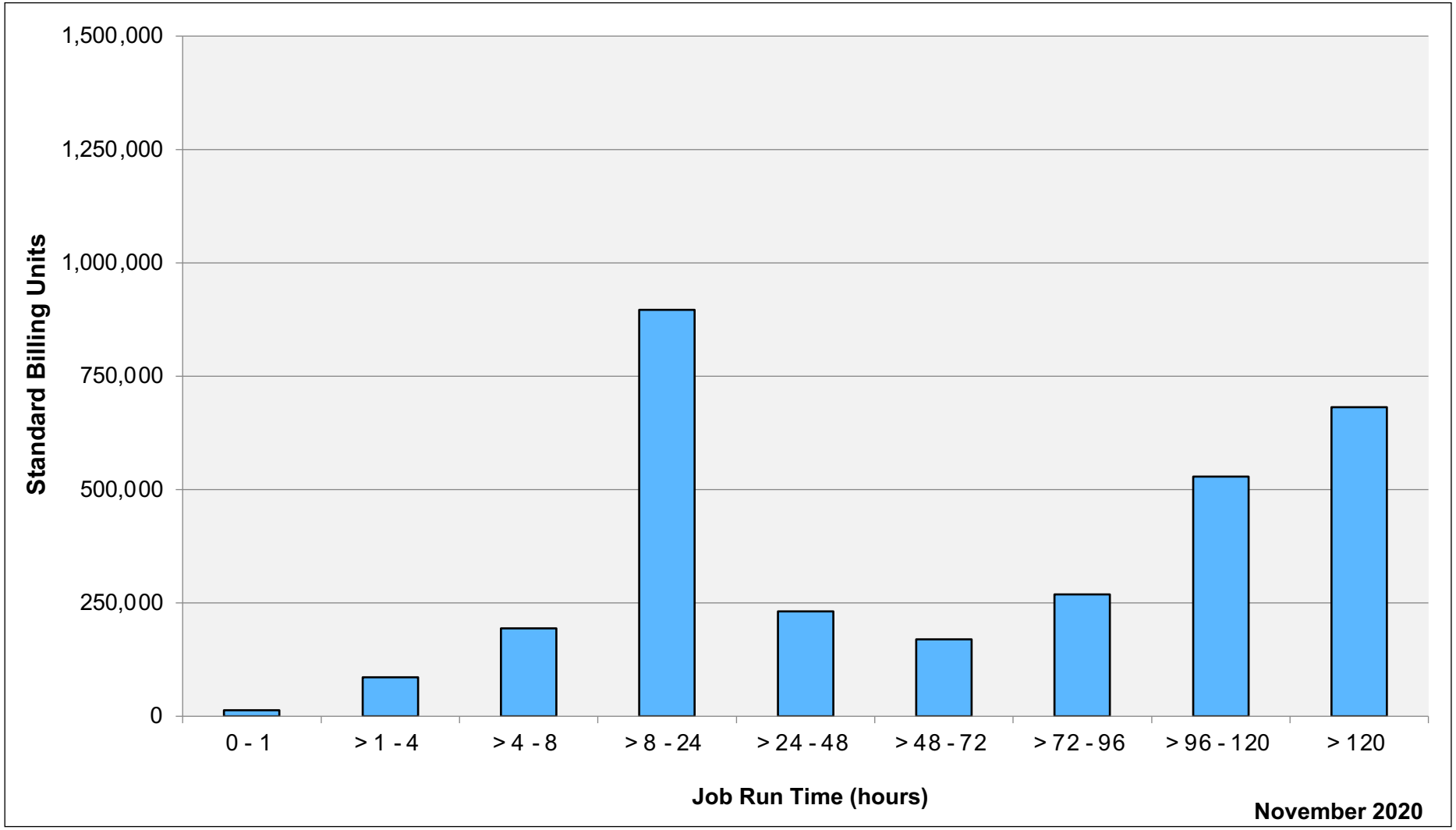
Electra: SBUs Reported, Normalized to 30-Day Month



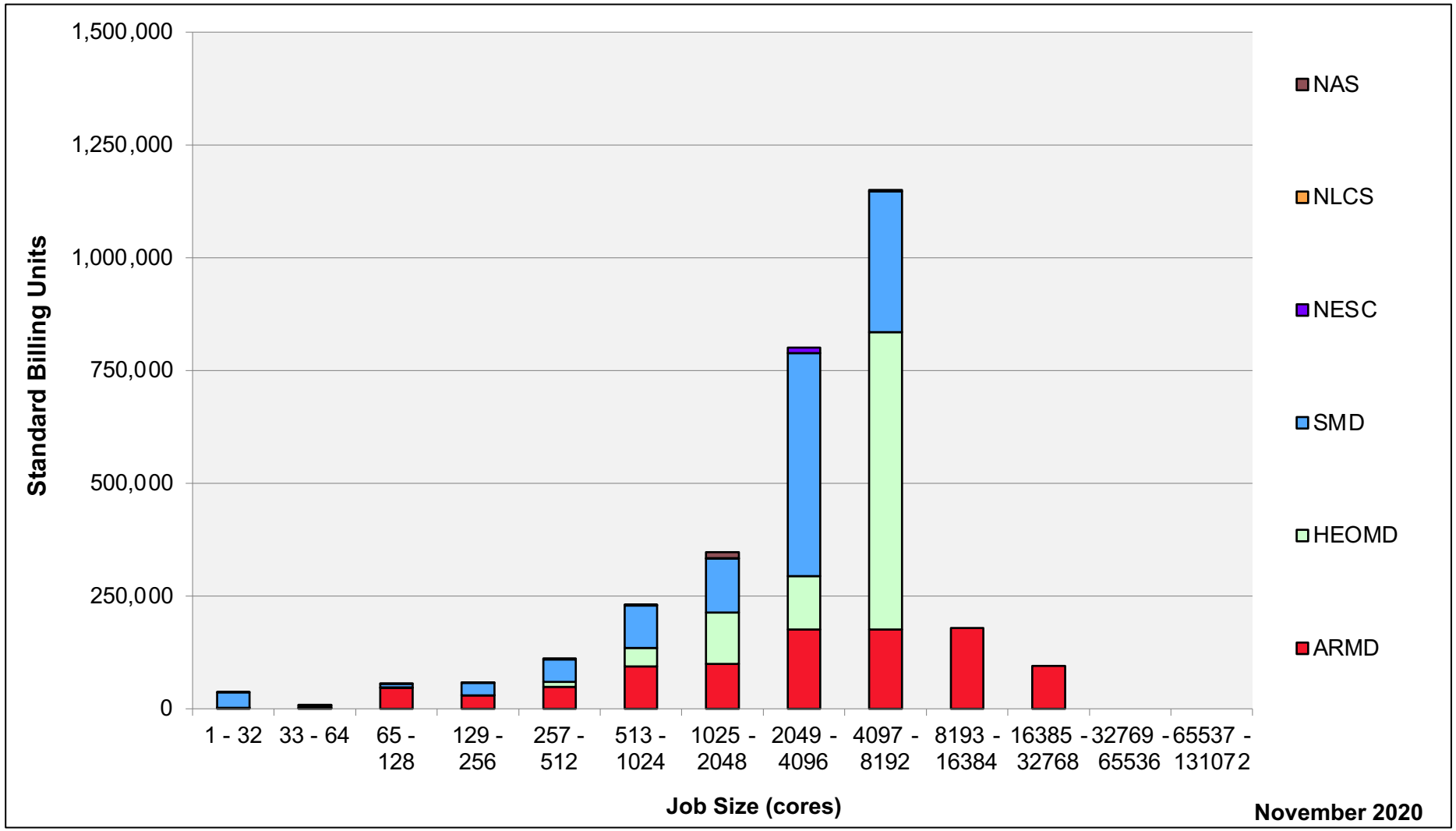
Electra: Devel Queue Utilization



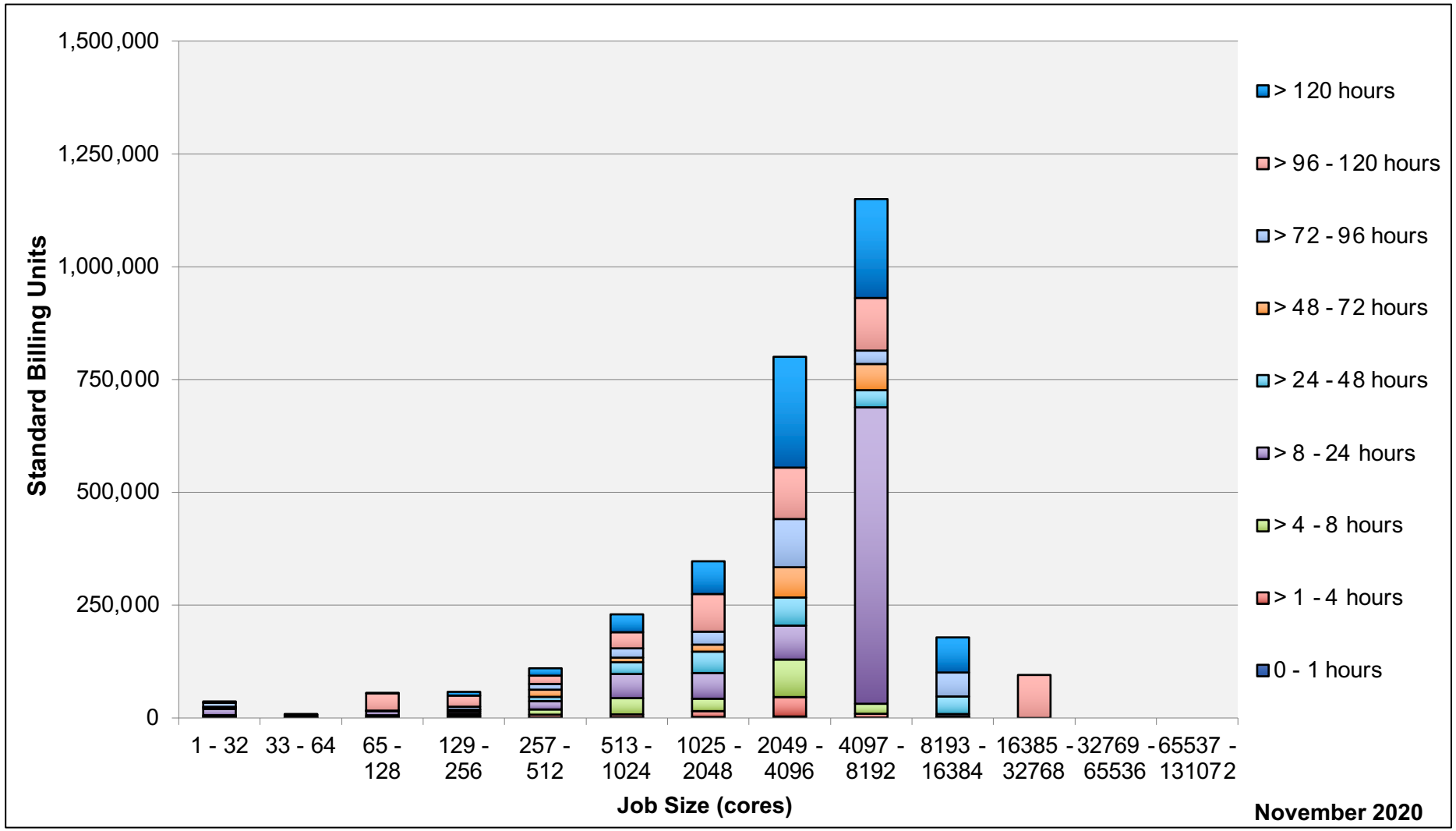
Electra: Monthly Utilization by Job Length



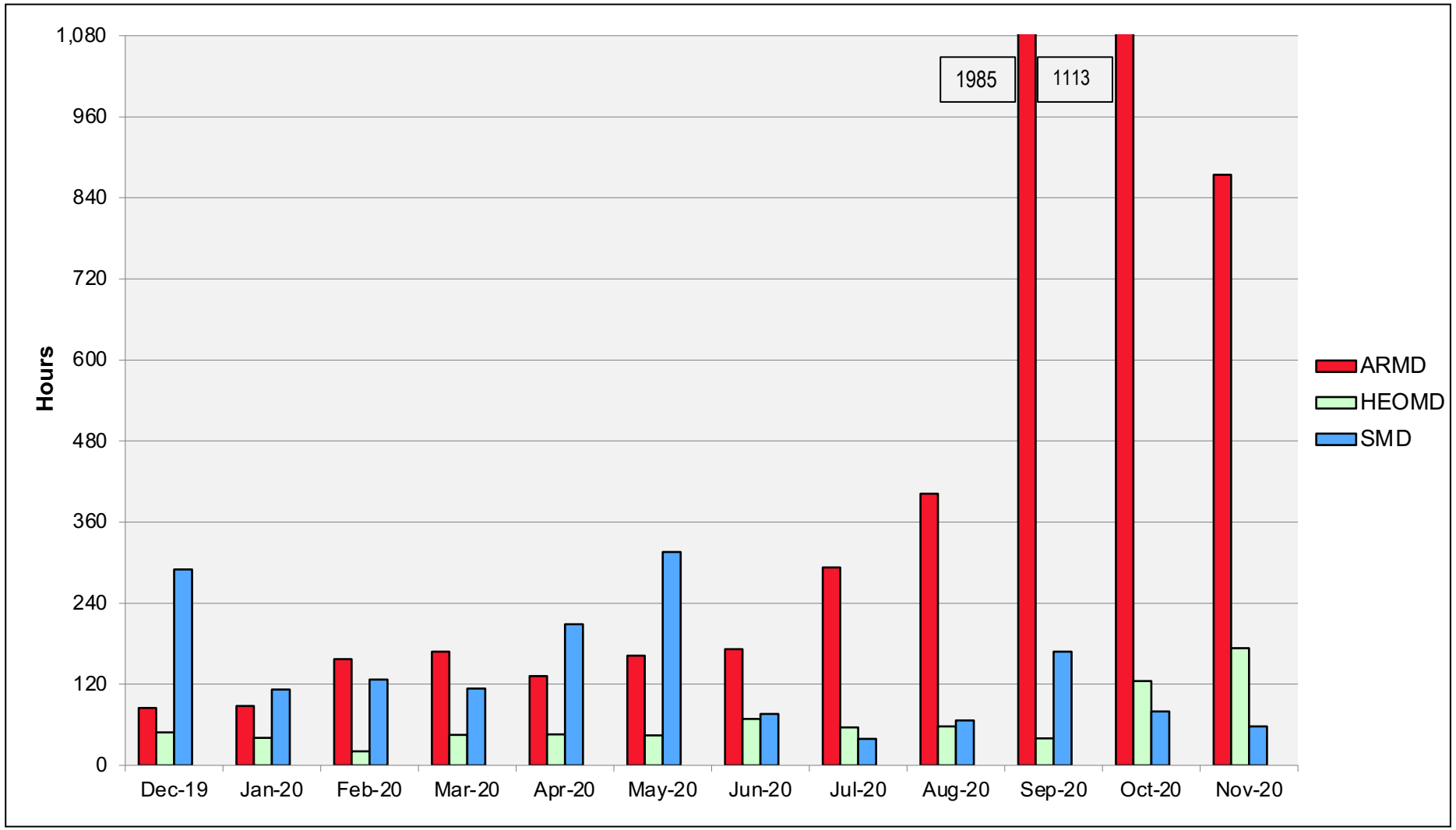
Electra: Monthly Utilization by Job Size



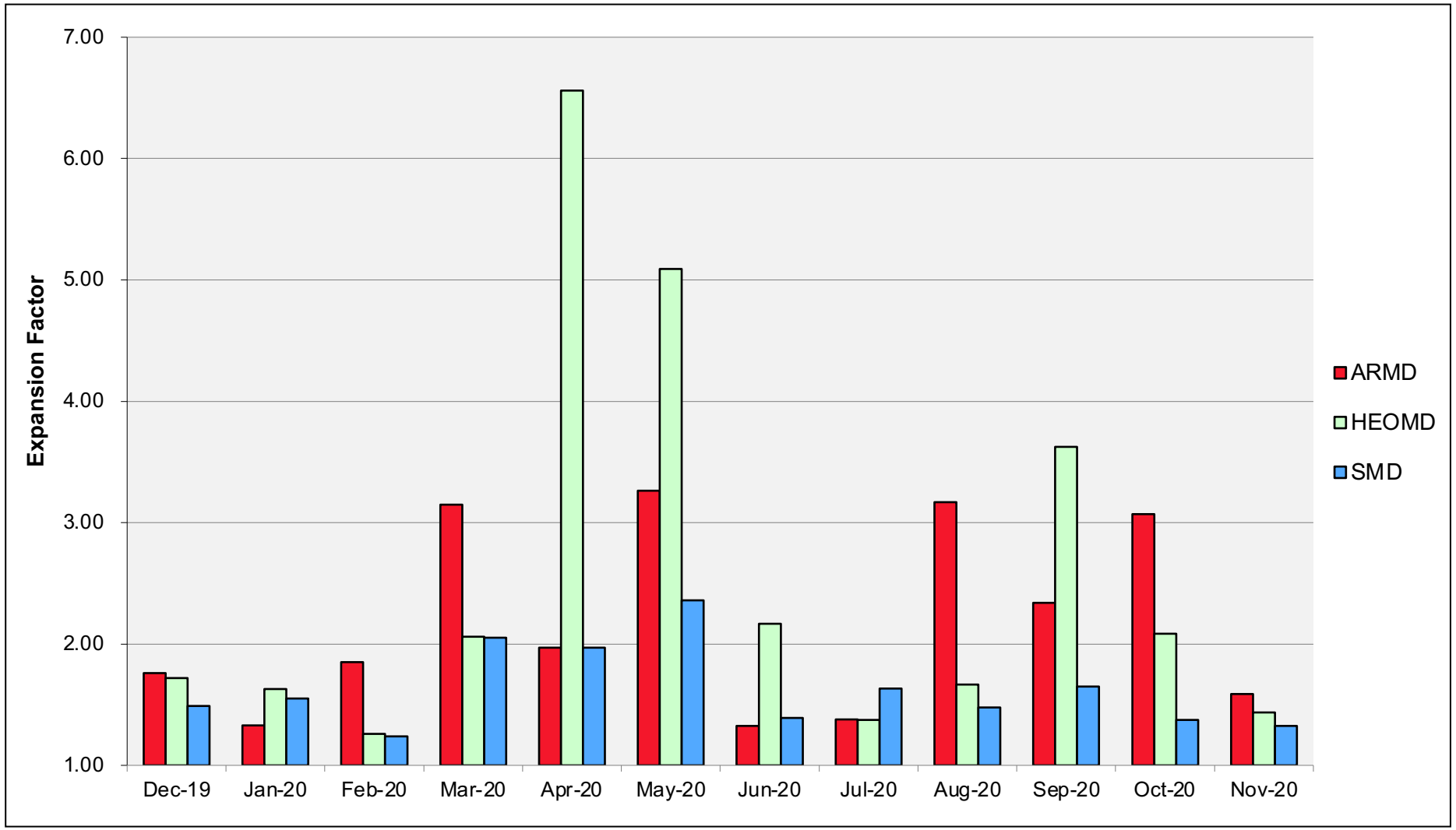
Electra: Monthly Utilization by Size and Length



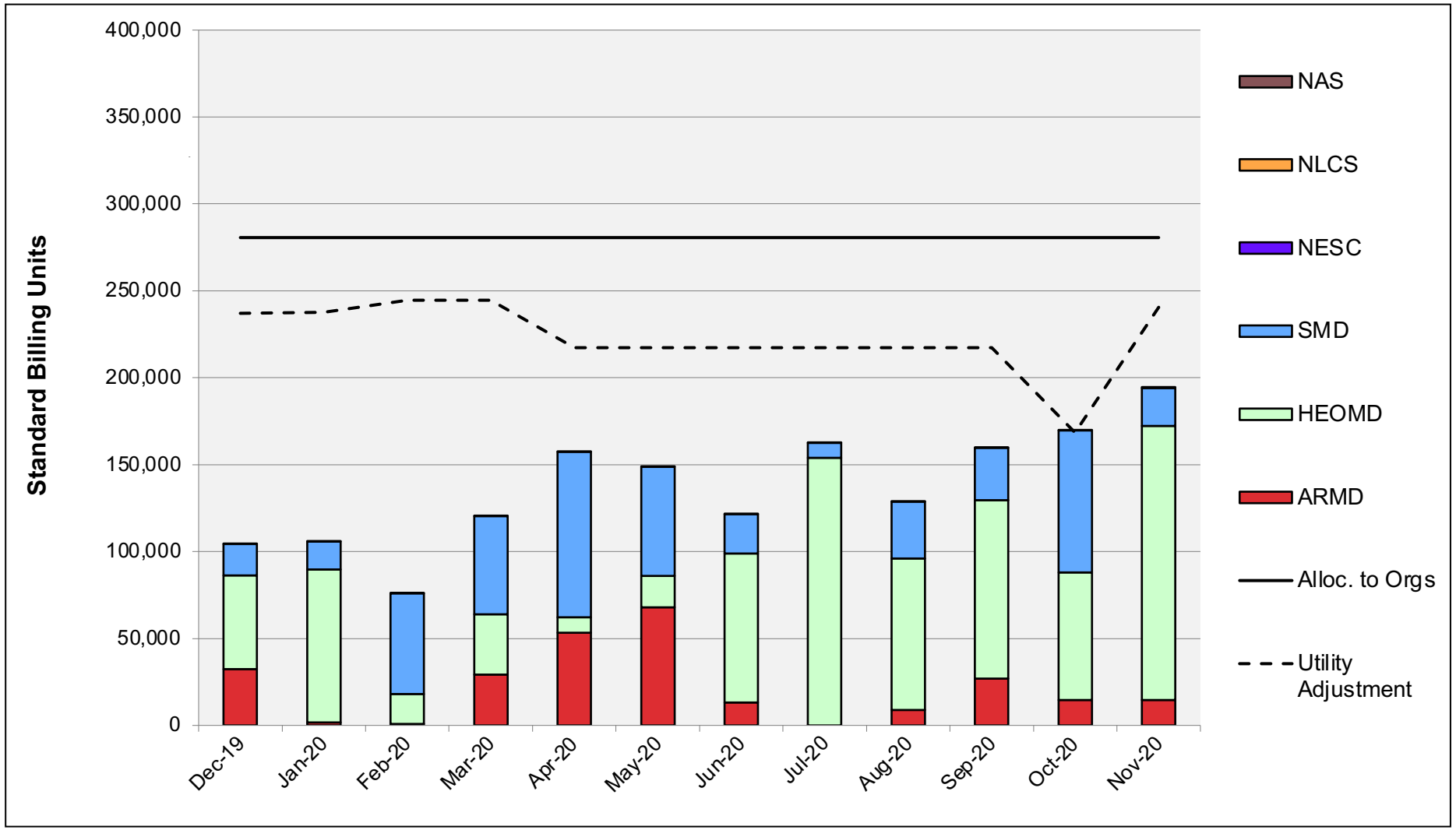
Electra: Average Time to Clear All Jobs



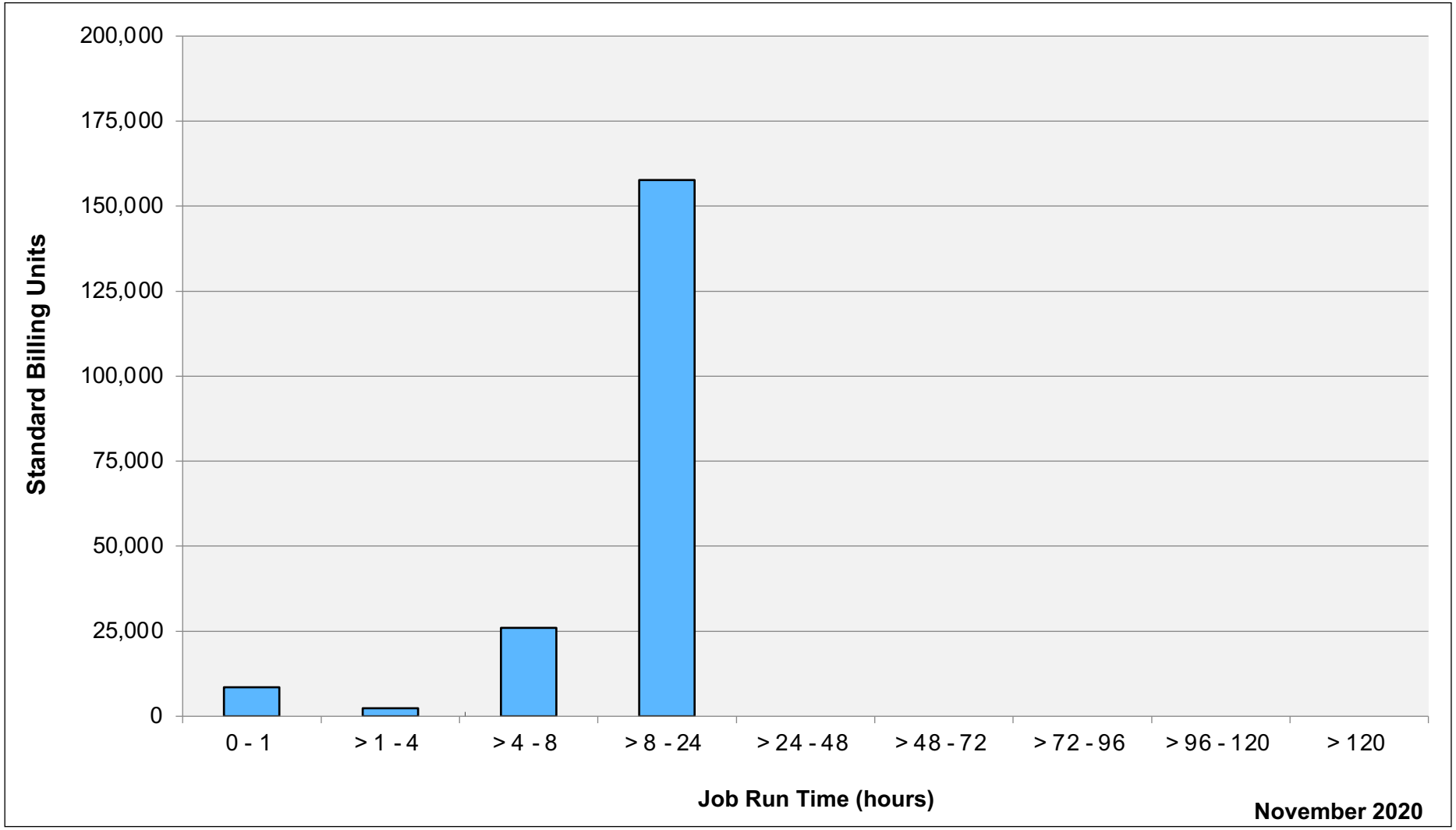
Electra: Average Expansion Factor



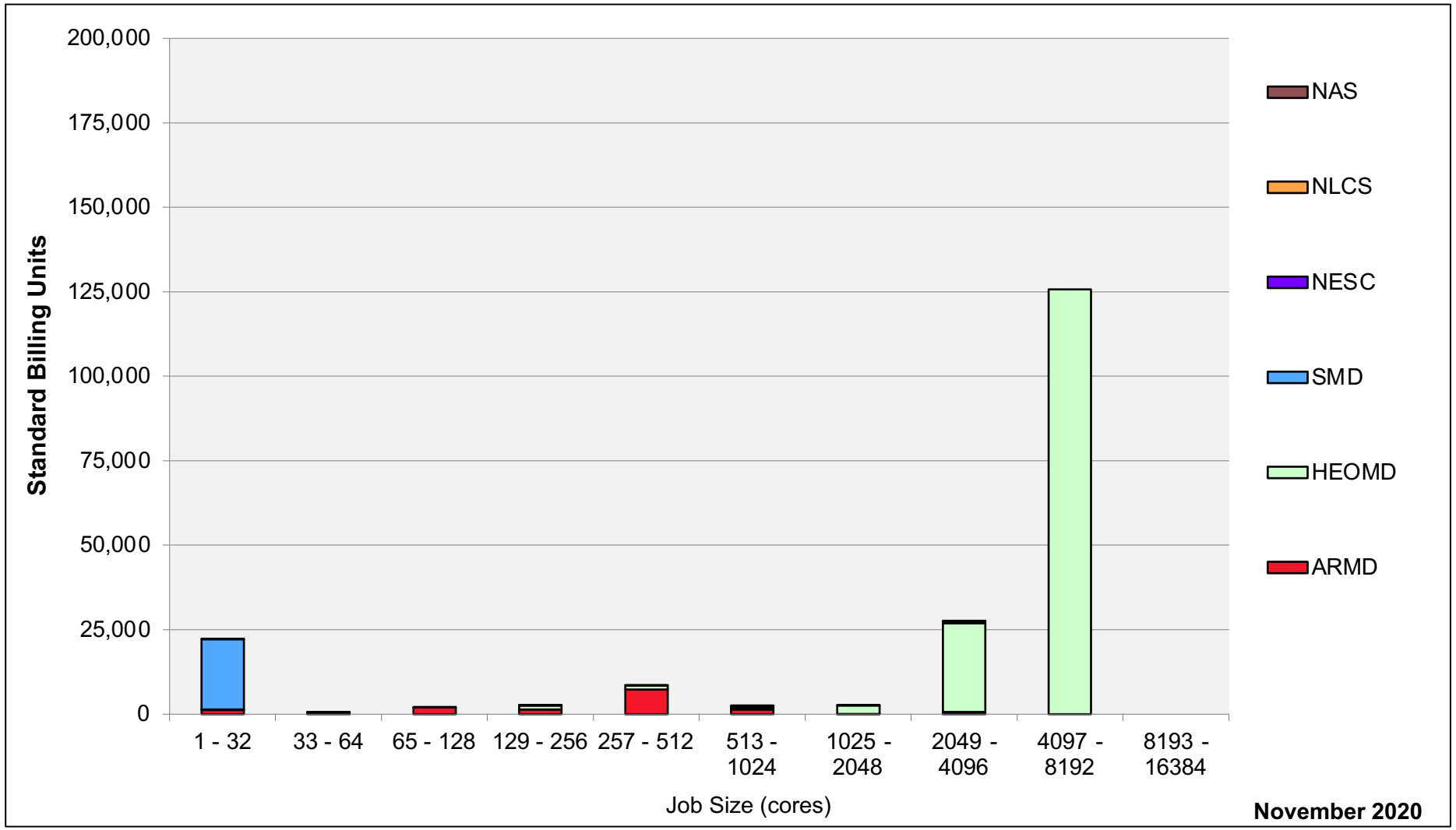
Merope: SBUs Reported, Normalized to 30-Day Month



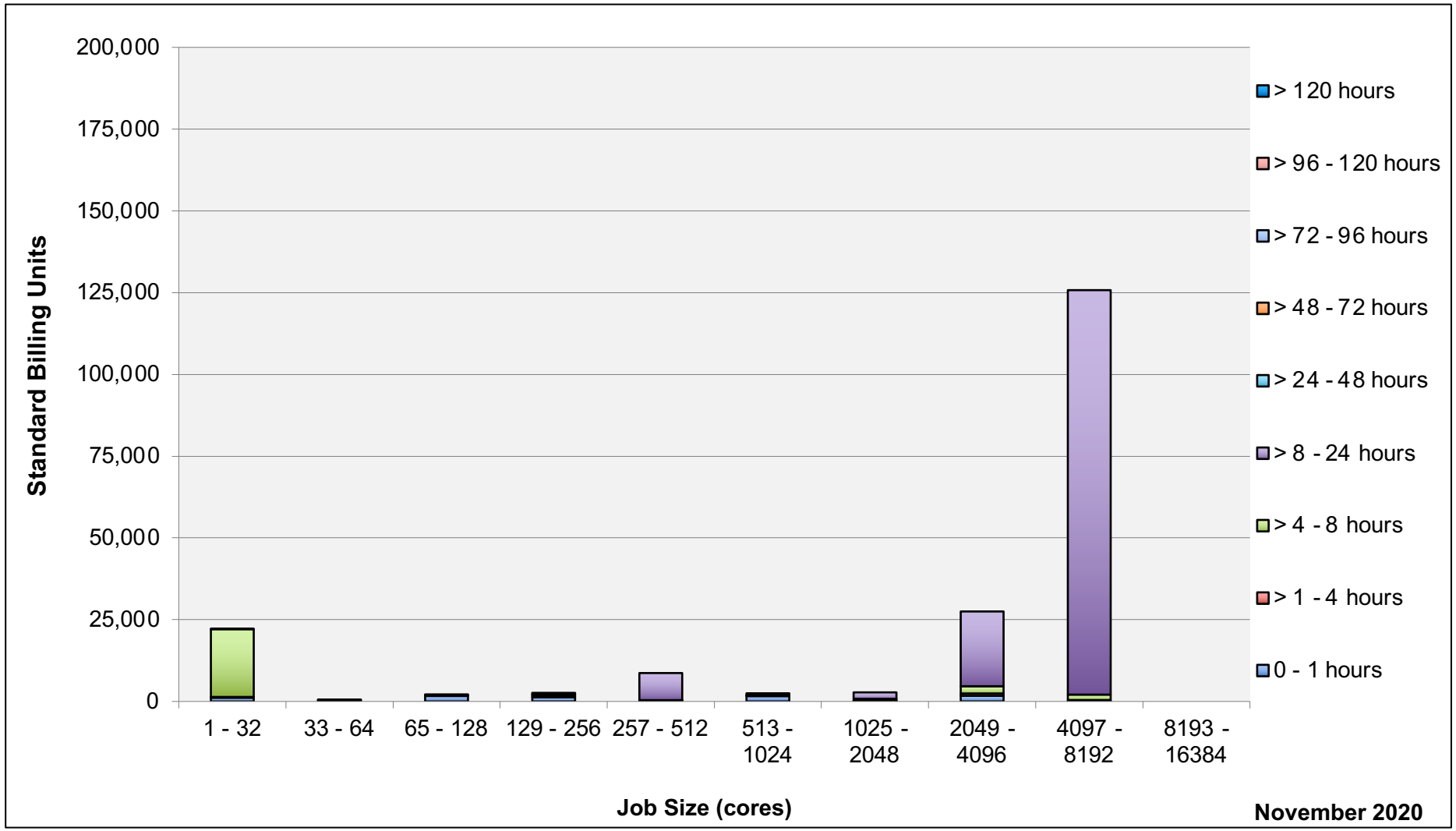
Merope: Monthly Utilization by Job Length



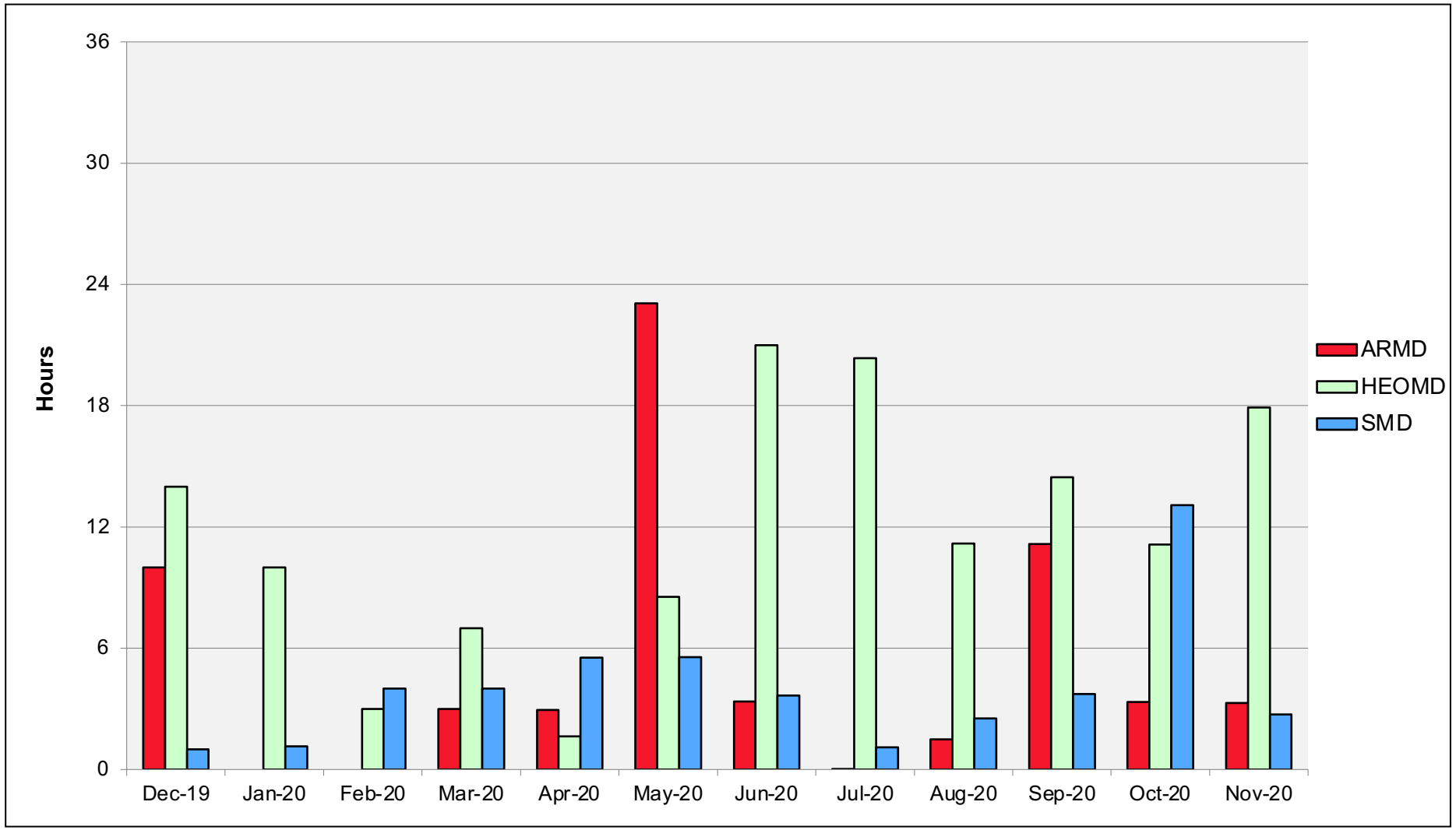
Merope: Monthly Utilization by Job Size



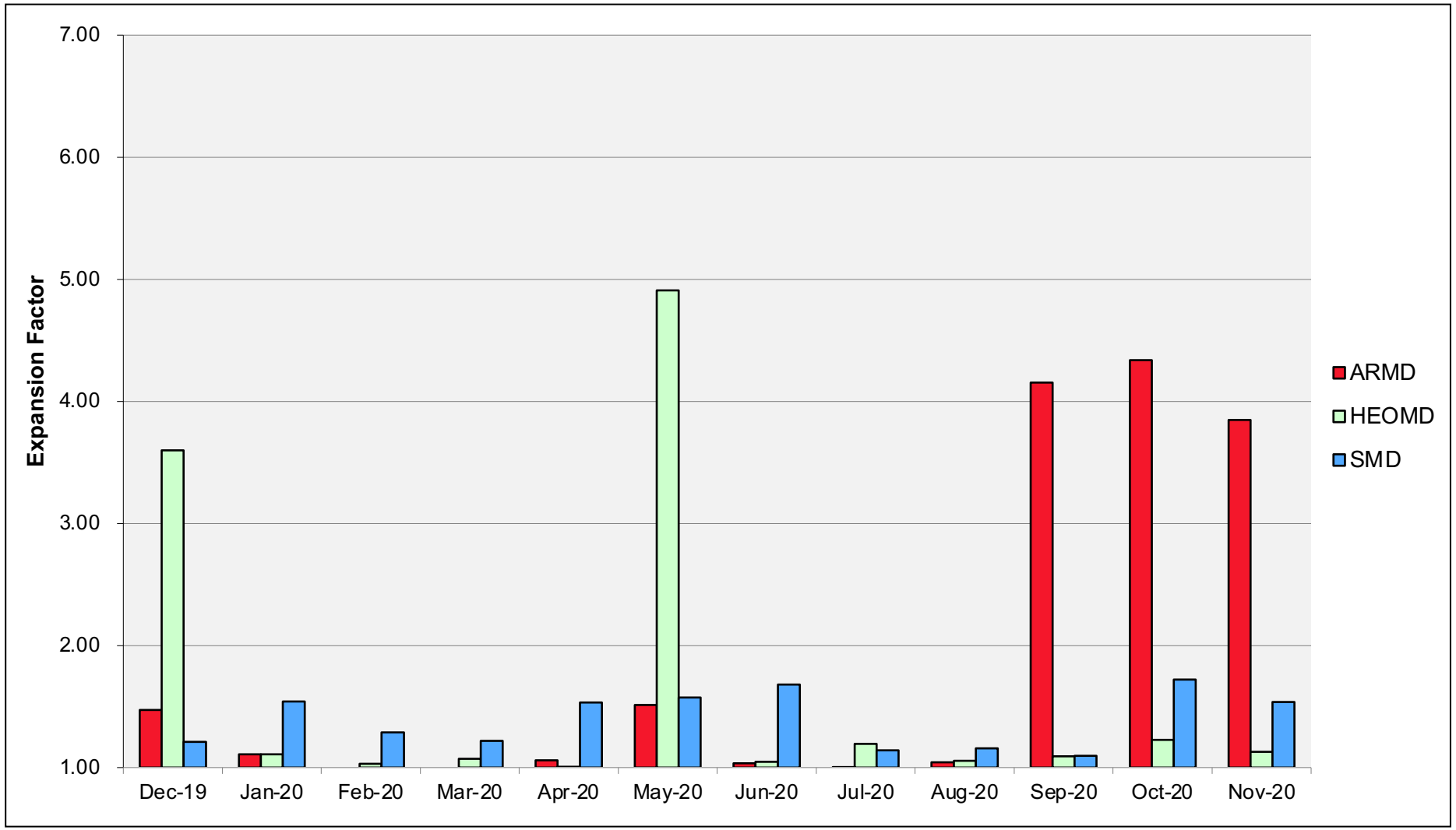
Merope: Monthly Utilization by Size and Length



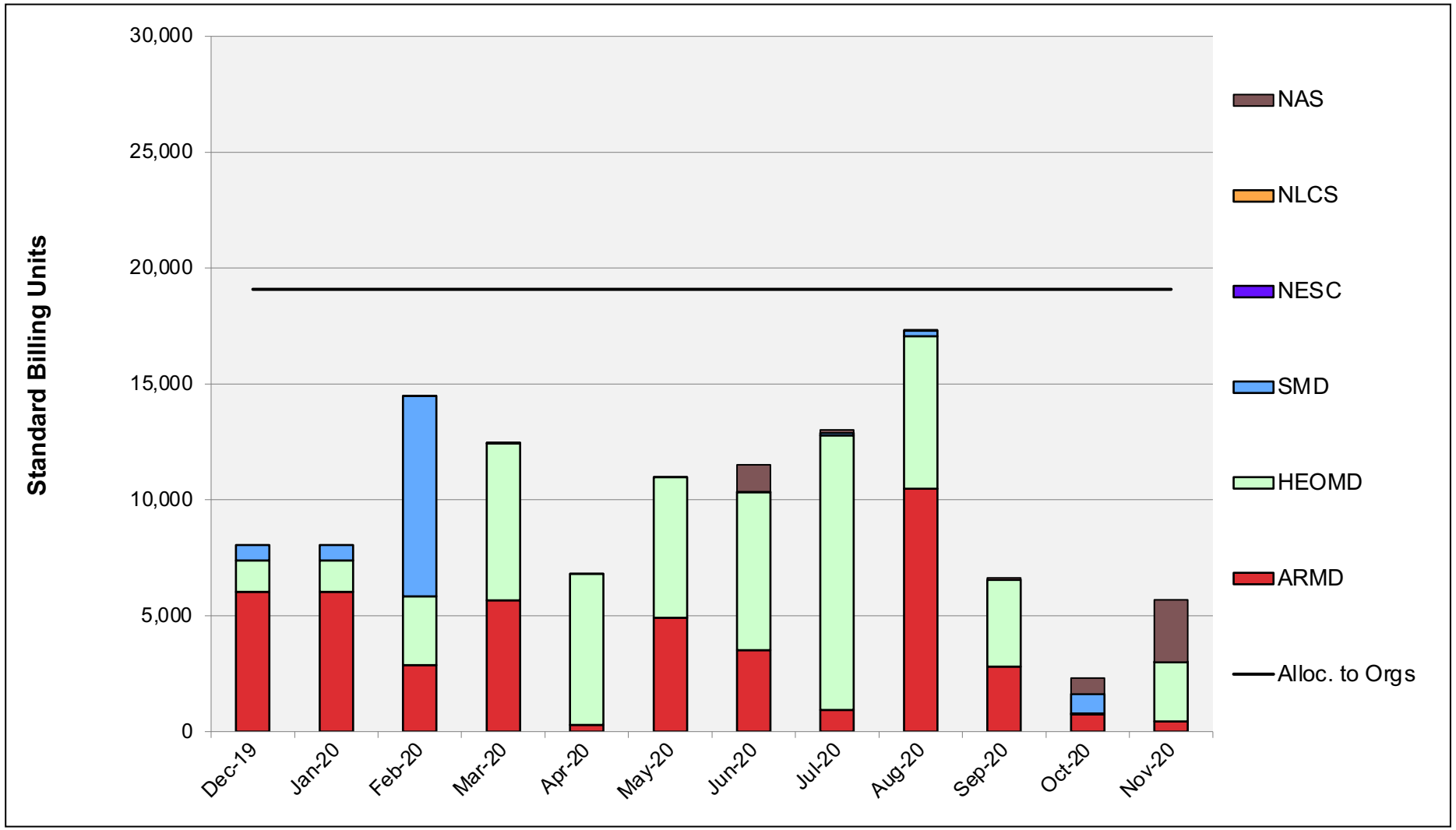
Merope: Average Time to Clear All Jobs



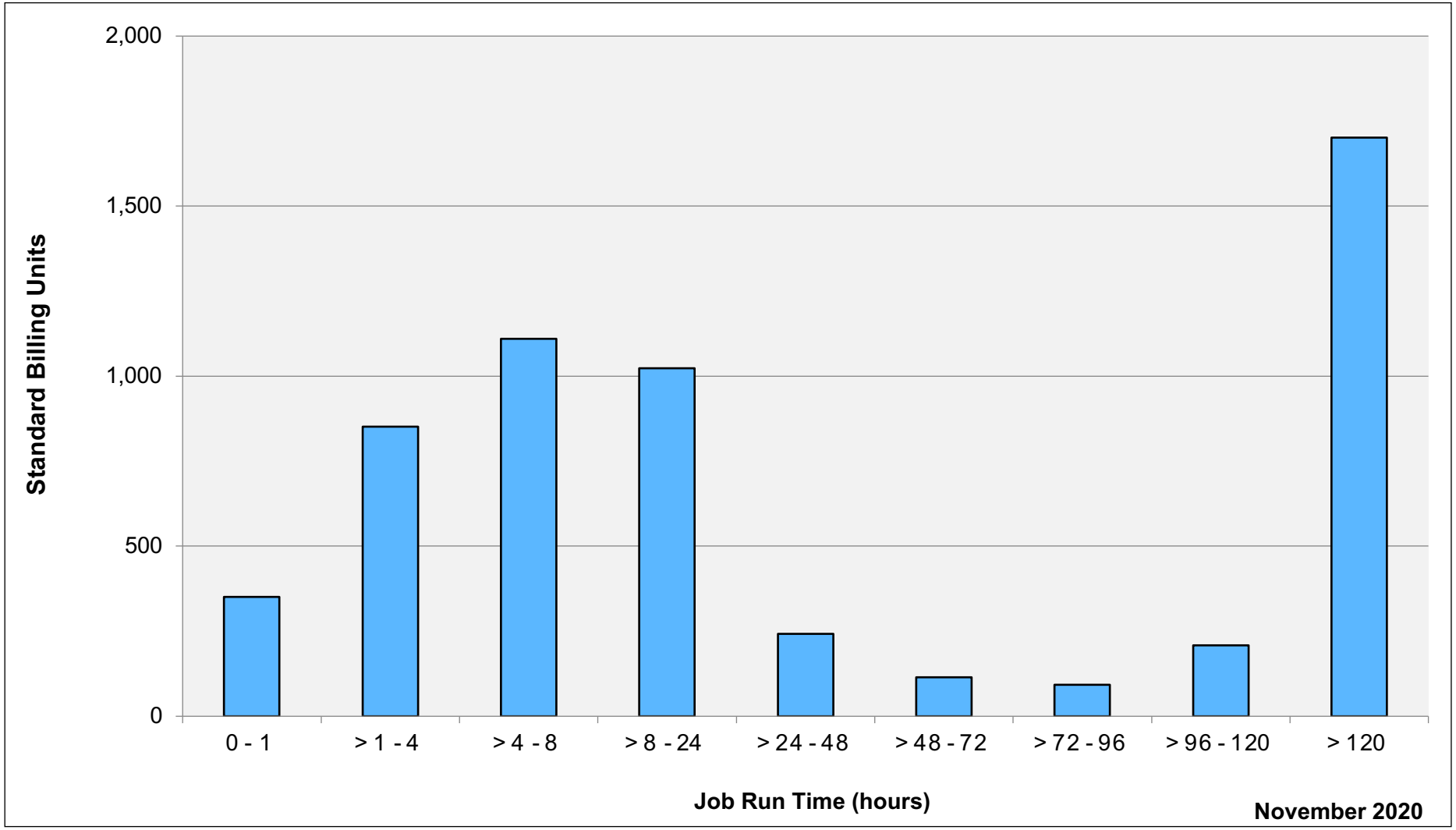
Merope: Average Expansion Factor



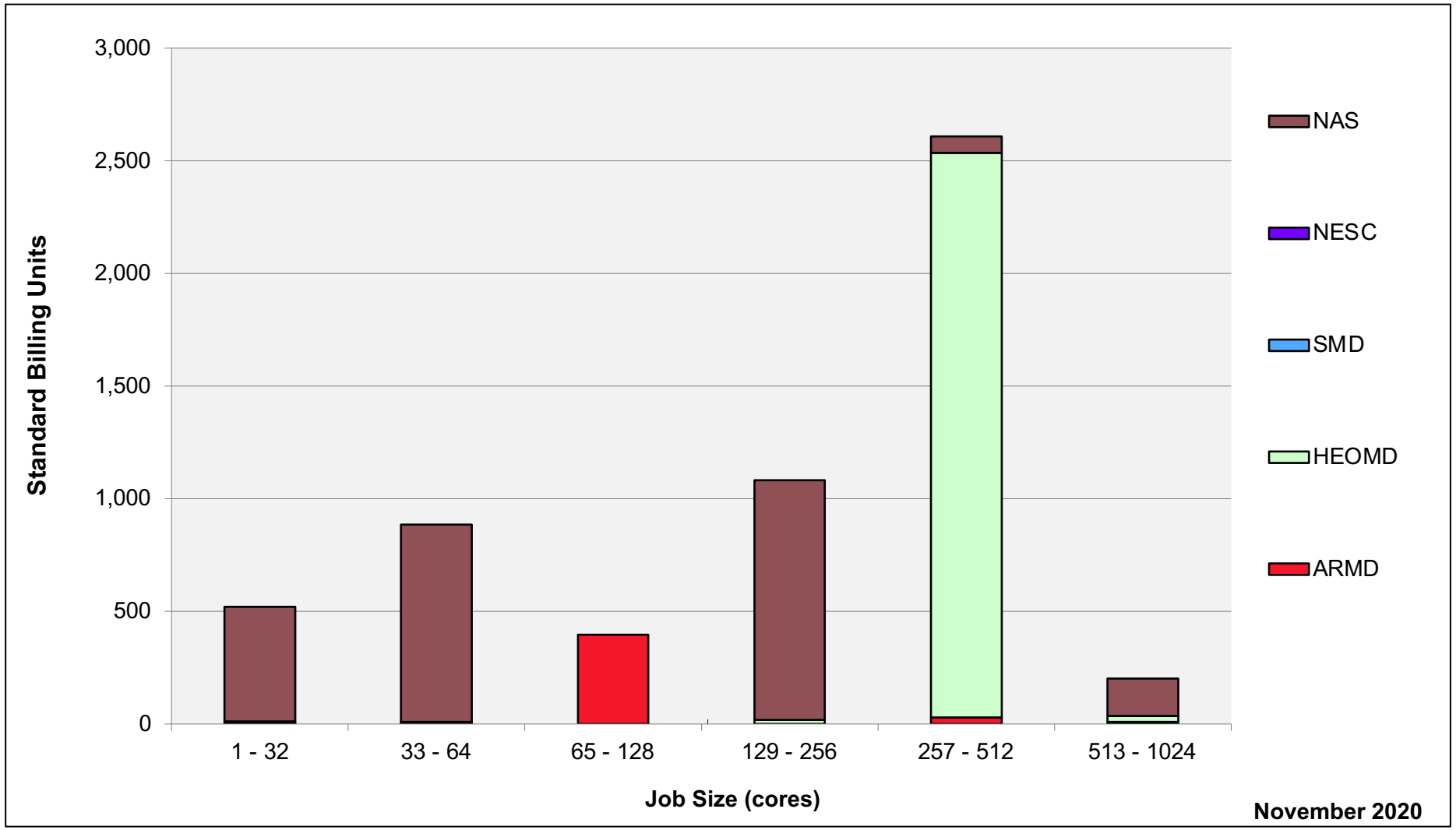
Endeavour: SBUs Reported, Normalized to 30-Day Month



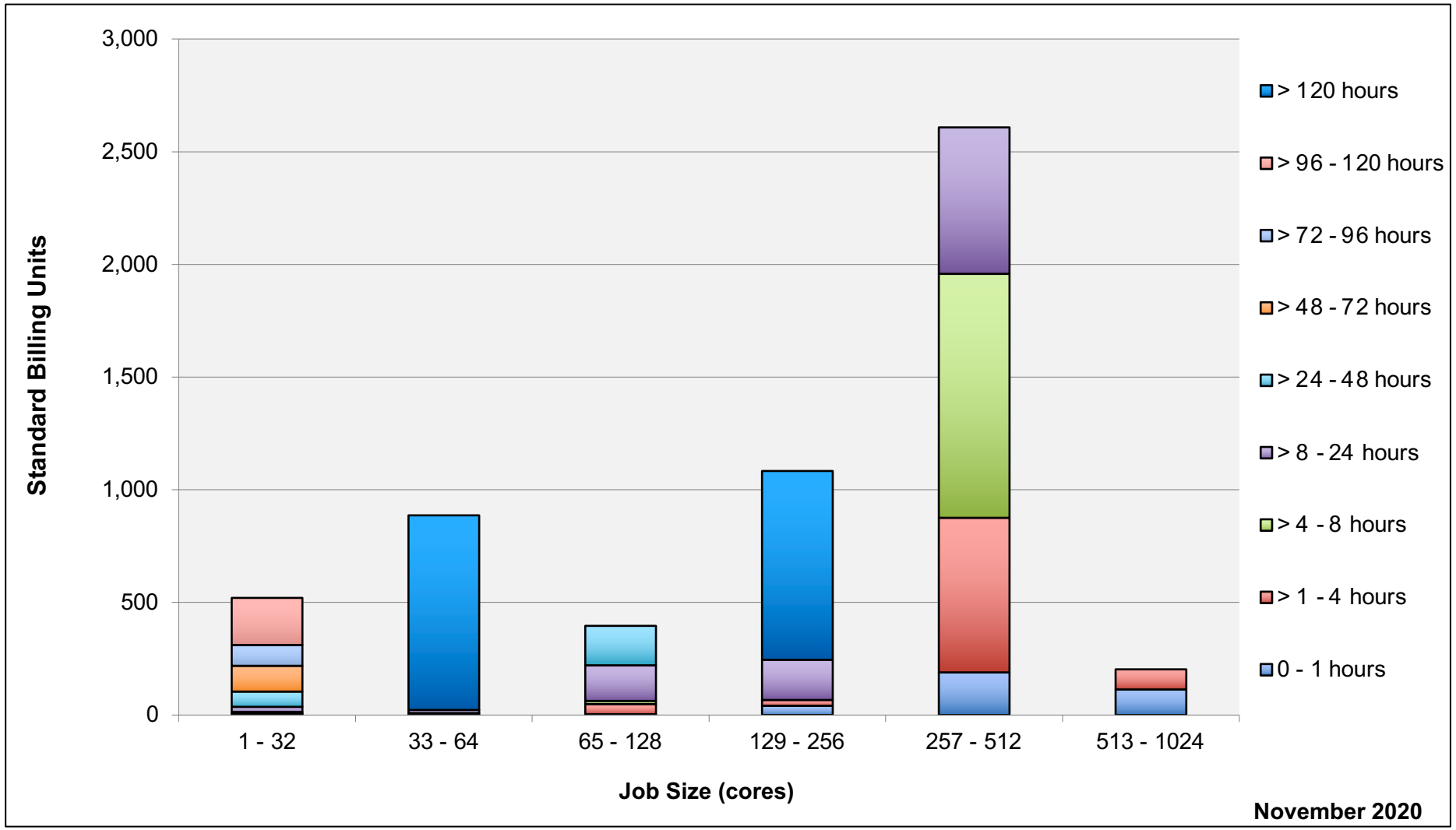
Endeavour: Monthly Utilization by Job Length



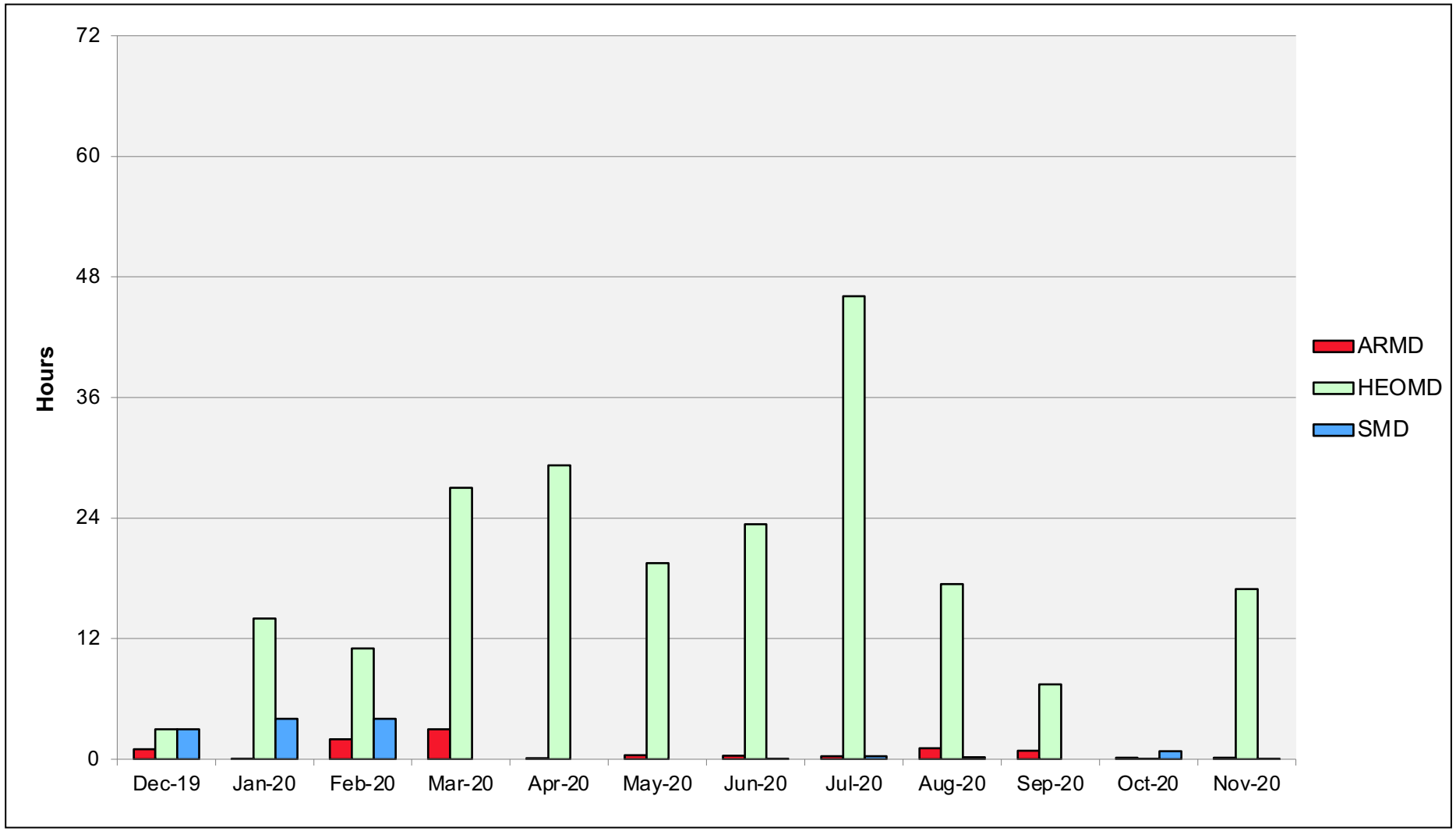
Endeavour: Monthly Utilization by Job Size



Endeavour: Monthly Utilization by Size and Length



Endeavour: Average Time to Clear All Jobs



Endeavour: Average Expansion Factor